



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 4FZC / pdb_00004fzc
Title : 20S yeast proteasome in complex with cepafungin I
Authors : Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on : 2012-07-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

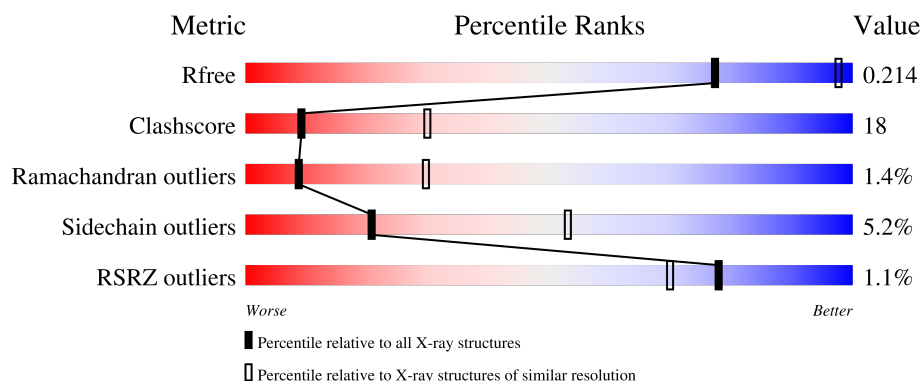
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	2% 66% 30% .
1	O	250	% 67% 30% .
2	B	244	2% 60% 34% 7%
2	P	244	3% 60% 34% 7%
3	C	241	3% 61% 35% 5%

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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	233	
13	a	233	
14	N	196	
14	b	196	
15	c	4	
15	d	4	

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Mol	Chain	Length	Quality of chain
15	e	4	 50%50%
15	f	4	 75%25%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Cepafungin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	d	4	Total	C	N	O	0	0	0
			38	28	4	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	f	4	Total	C	N	O	0	0	0
			38	28	4	6			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	37	Total	O	0	0
			37	37		
16	C	41	Total	O	0	0
			41	41		
16	D	40	Total	O	0	0
			40	40		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	59	Total	O	0	0
			59	59		
16	H	53	Total	O	0	0
			53	53		
16	I	68	Total	O	0	0
			68	68		
16	J	51	Total	O	0	0
			51	51		
16	K	43	Total	O	0	0
			43	43		
16	L	58	Total	O	0	0
			58	58		
16	M	71	Total	O	0	0
			71	71		
16	N	58	Total	O	0	0
			58	58		
16	O	33	Total	O	0	0
			33	33		
16	P	27	Total	O	0	0
			27	27		
16	Q	26	Total	O	0	0
			26	26		

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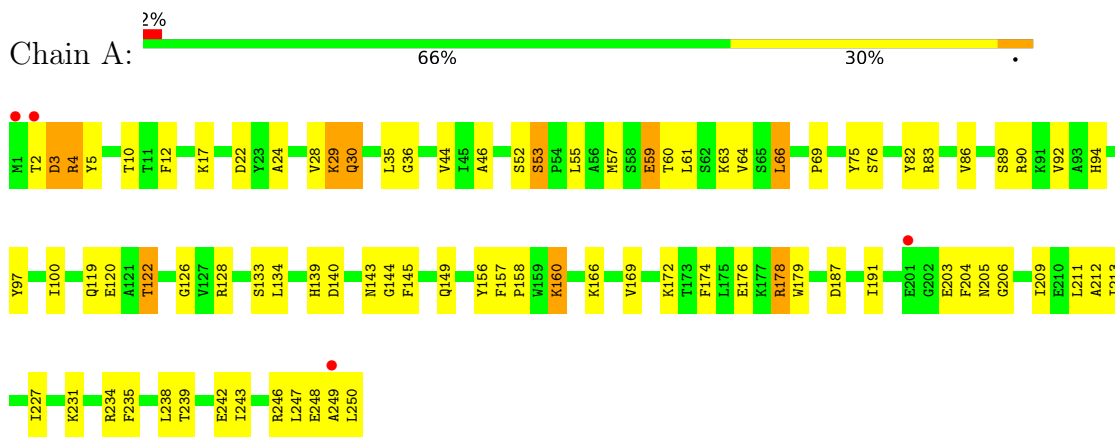
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	28	Total 28	O 28	0	0
16	S	21	Total 21	O 21	0	0
16	T	38	Total 38	O 38	0	0
16	U	62	Total 62	O 62	0	0
16	V	47	Total 47	O 47	0	0
16	W	57	Total 57	O 57	0	0
16	X	47	Total 47	O 47	0	0
16	Y	41	Total 41	O 41	0	0
16	Z	55	Total 55	O 55	0	0
16	a	74	Total 74	O 74	0	0
16	b	60	Total 60	O 60	0	0
16	f	1	Total 1	O 1	0	0

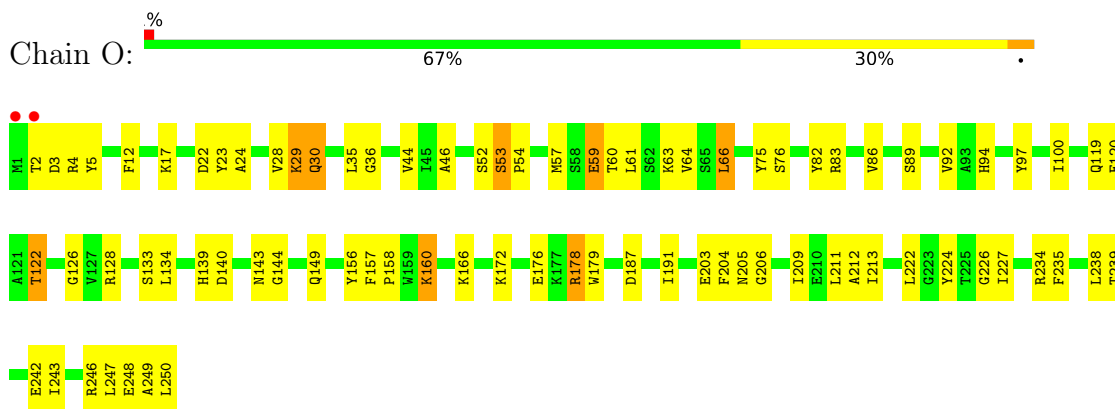
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

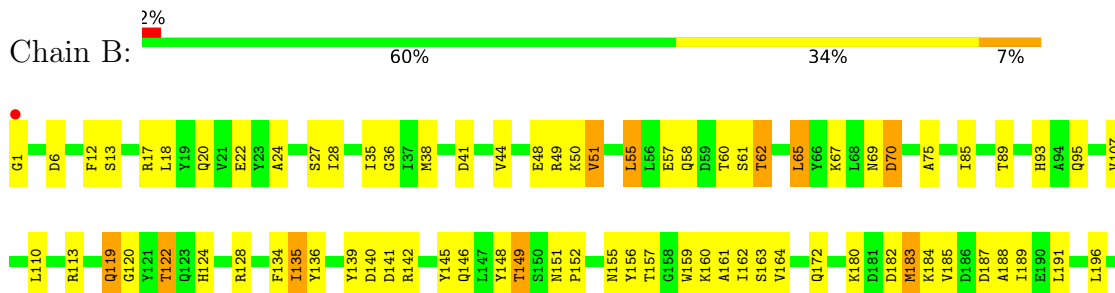
- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

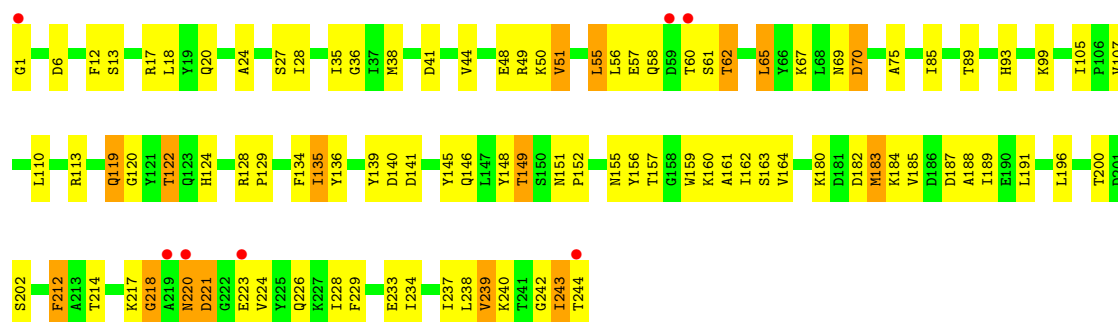


- Molecule 2: Proteasome component Y13

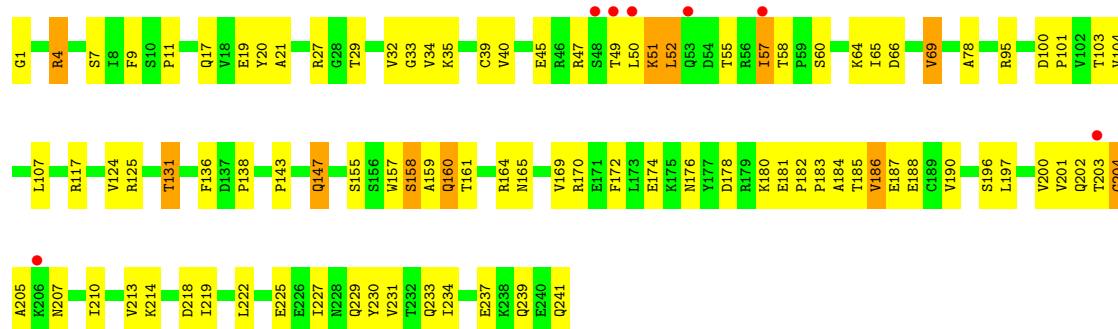




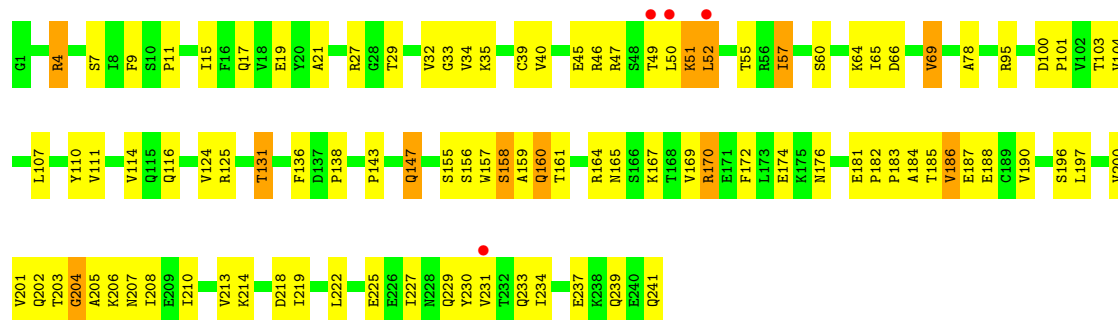
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

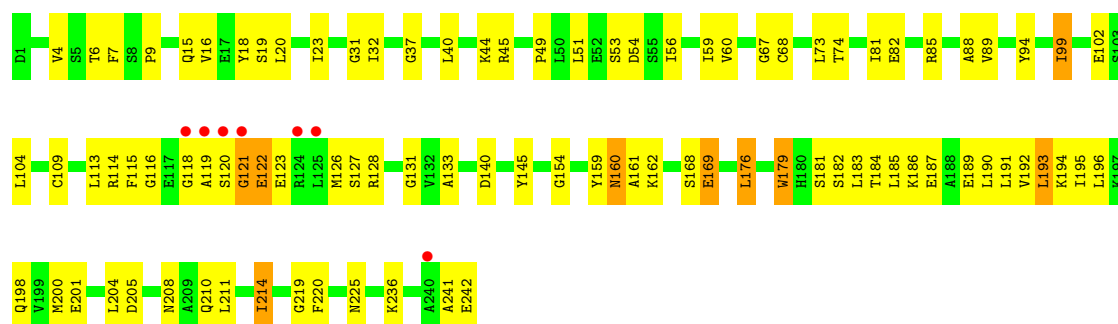


• Molecule 3: Proteasome component PRE6

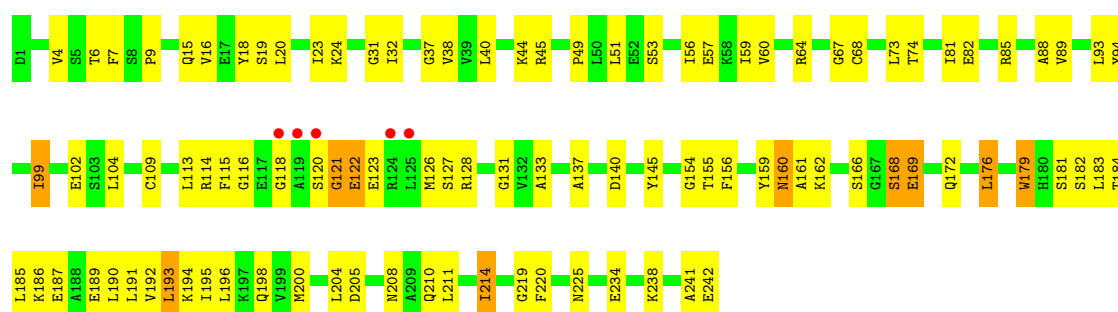


• Molecule 4: Proteasome component PUP2

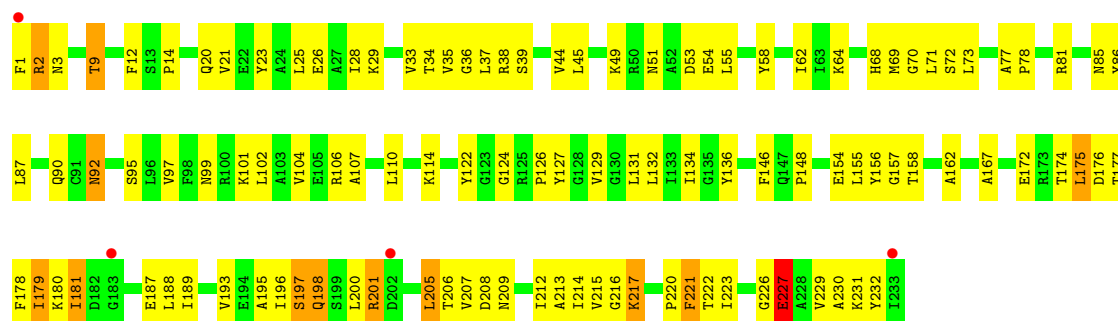




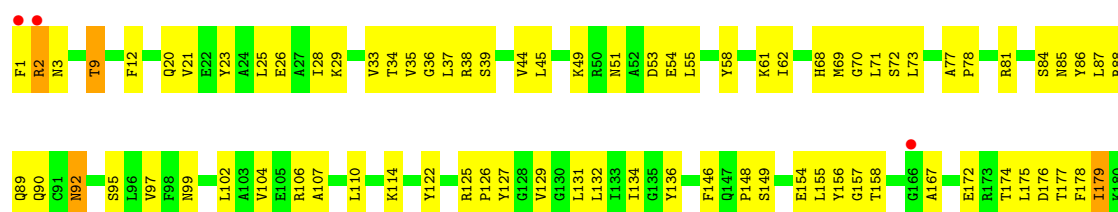
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5

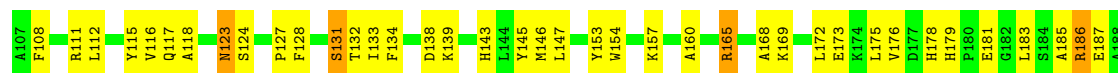


• Molecule 5: Proteasome component PRE5

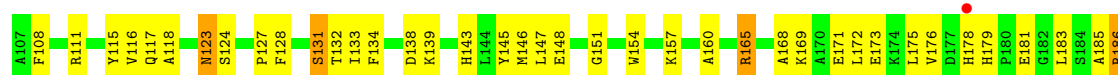
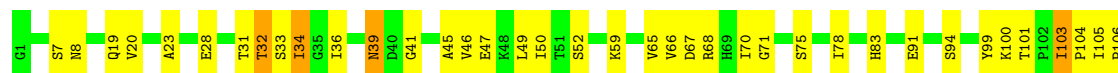




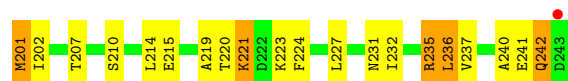
• Molecule 6: Proteasome component C1



• Molecule 6: Proteasome component C1

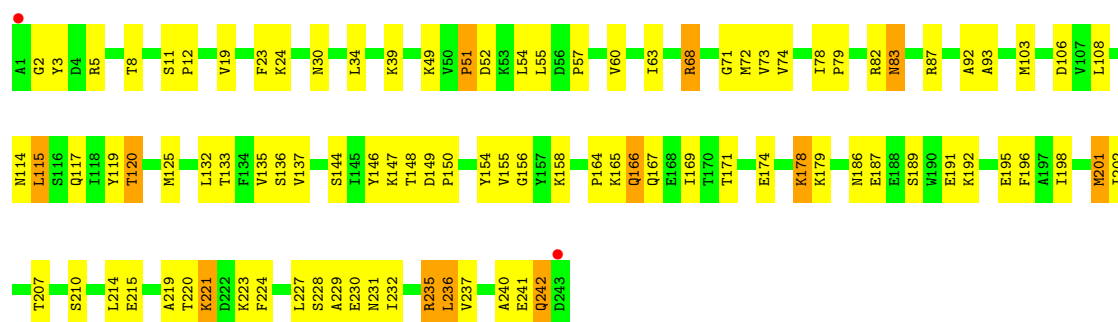


• Molecule 7: Proteasome component C7-alpha



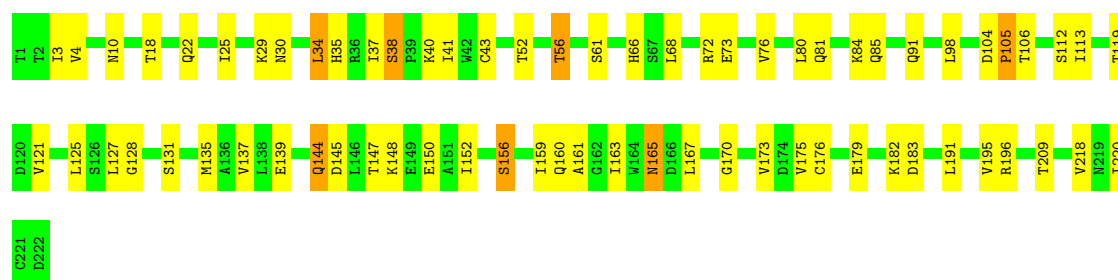
• Molecule 7: Proteasome component C7-alpha





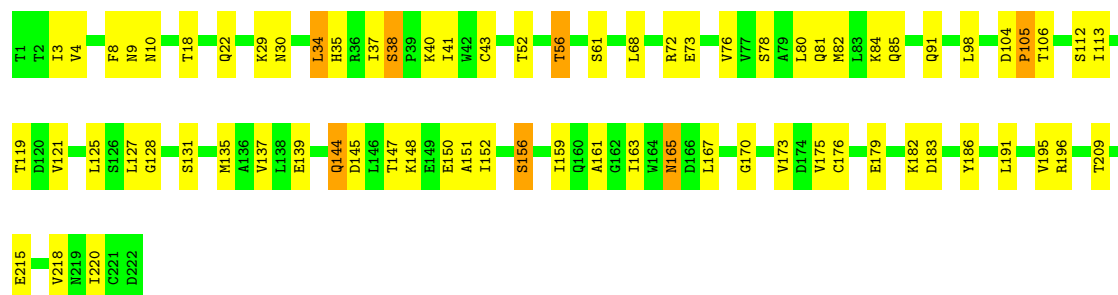
• Molecule 8: Proteasome component PUP1

Chain H: 69% 28%



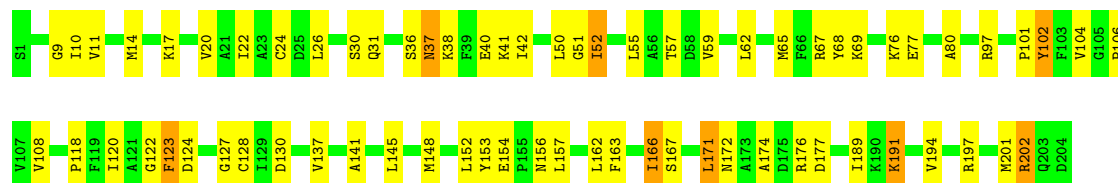
• Molecule 8: Proteasome component PUP1

Chain V: 67% 30%



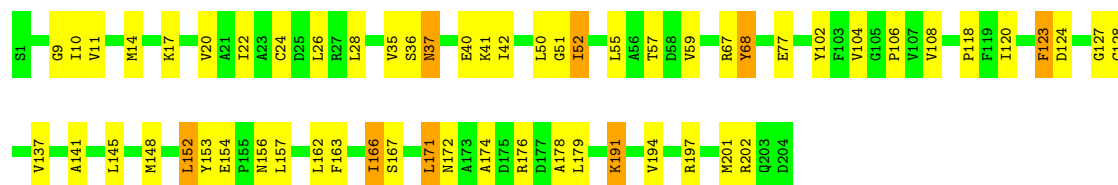
• Molecule 9: Proteasome component PUP3

Chain I: 66% 30%

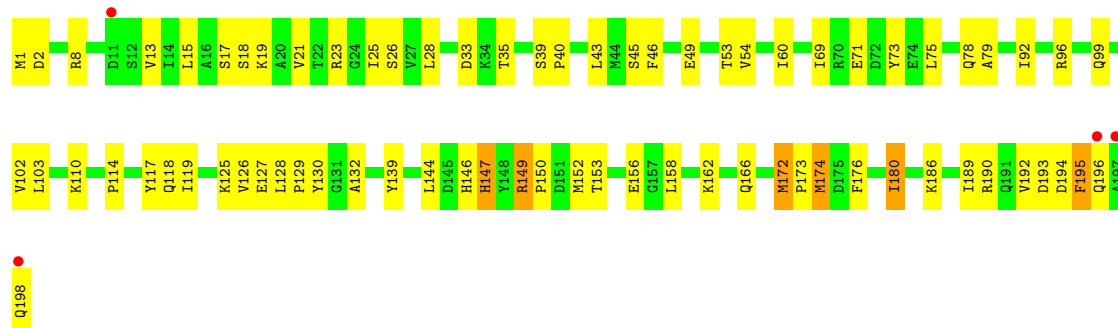


• Molecule 9: Proteasome component PUP3

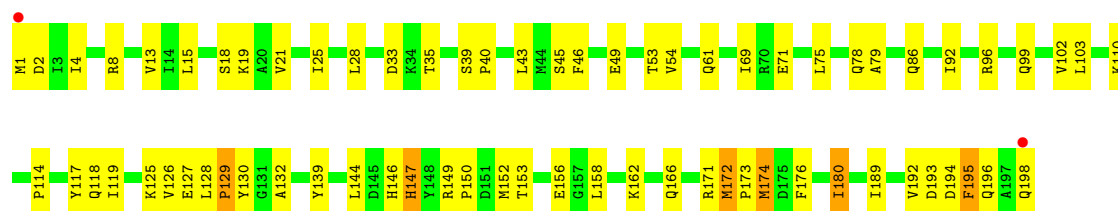
Chain W: 71% 25%



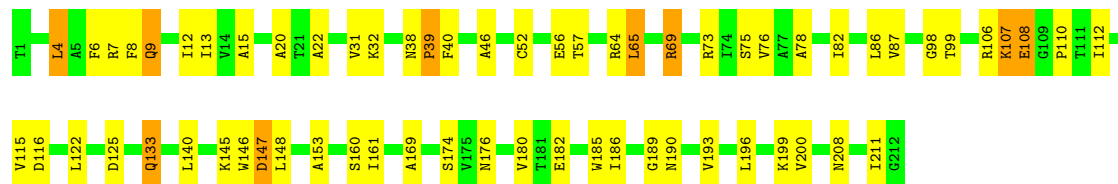
- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11



- Molecule 11: Proteasome component PRE2



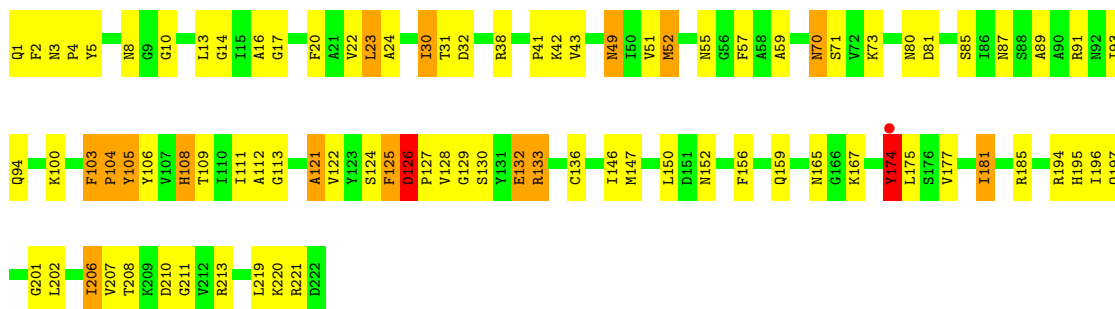
- Molecule 11: Proteasome component PRE2





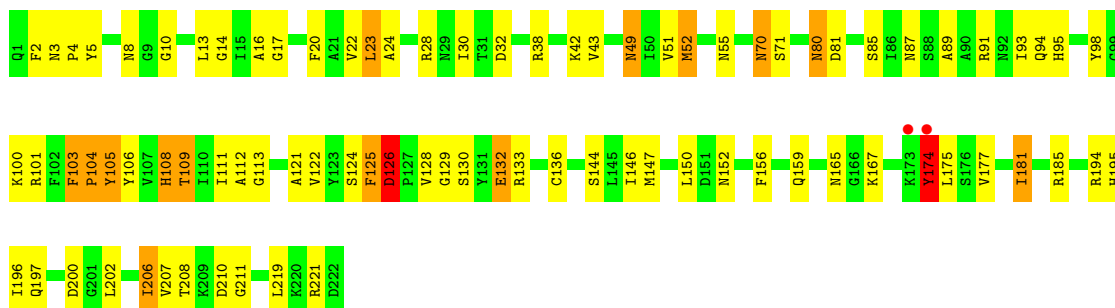
• Molecule 12: Proteasome component C5

Chain L: 60% 32% 7% .



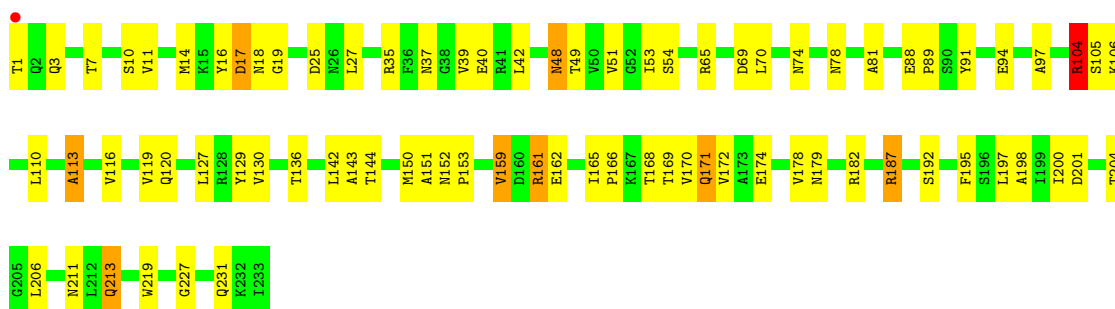
• Molecule 12: Proteasome component C5

Chain Z: 62% 31% 6% .



• Molecule 13: Proteasome component PRE4

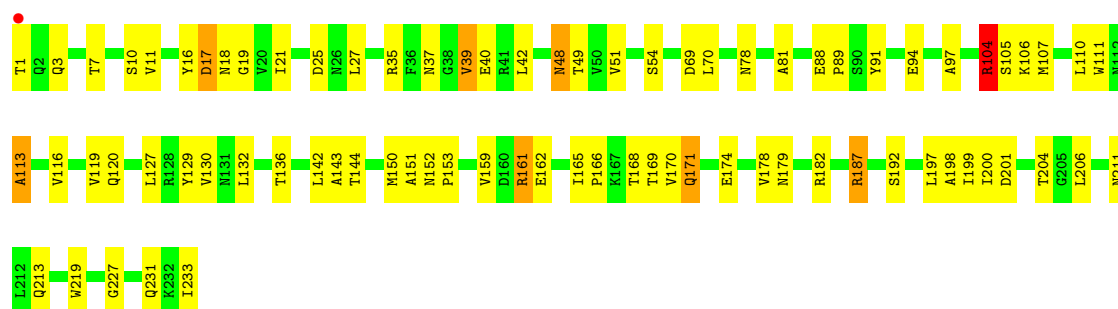
Chain M: 66% 30% .



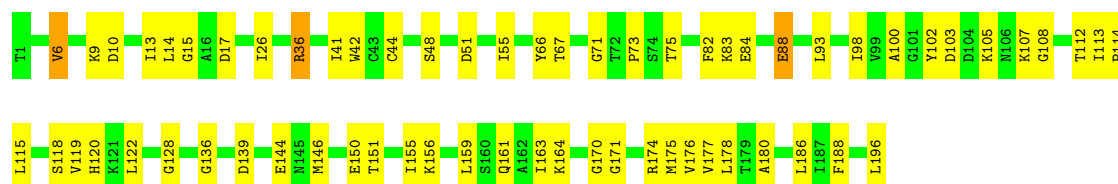
• Molecule 13: Proteasome component PRE4

Chain a: 66% 31% .

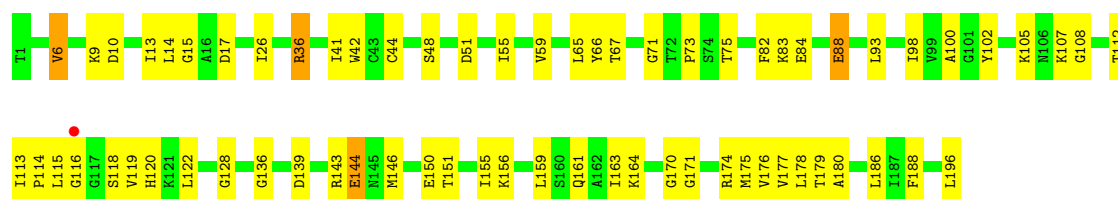




• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



• Molecule 15: Cepafungin I



• Molecule 15: Cepafungin I



• Molecule 15: Cepafungin I



- Molecule 15: Cepafungin I

Chain f:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 301.02Å 144.83Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.80) 97.4 (15.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.244 0.214 , 0.214	Depositor DCC
R_{free} test set	12823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51020	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LYO, OW6, OW5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1952	0.95	7/2642 (0.3%)
1	O	0.42	0/1952	0.95	7/2642 (0.3%)
2	B	0.45	0/1935	0.92	6/2618 (0.2%)
2	P	0.46	0/1935	0.92	6/2618 (0.2%)
3	C	0.41	0/1920	0.93	7/2598 (0.3%)
3	Q	0.42	0/1920	0.94	8/2598 (0.3%)
4	D	0.41	0/1887	0.91	9/2541 (0.4%)
4	R	0.41	0/1887	0.92	8/2541 (0.3%)
5	E	0.41	0/1823	0.92	5/2463 (0.2%)
5	S	0.41	0/1823	0.93	6/2463 (0.2%)
6	F	0.44	0/1937	0.96	5/2614 (0.2%)
6	T	0.44	0/1937	0.96	6/2614 (0.2%)
7	G	0.46	0/1959	0.96	4/2652 (0.2%)
7	U	0.45	0/1959	0.95	5/2652 (0.2%)
8	H	0.46	0/1716	0.94	5/2326 (0.2%)
8	V	0.45	0/1716	0.95	4/2326 (0.2%)
9	I	0.46	0/1611	0.95	6/2174 (0.3%)
9	W	0.46	0/1611	0.96	5/2174 (0.2%)
10	J	0.47	0/1613	0.97	9/2173 (0.4%)
10	X	0.47	0/1613	0.98	10/2173 (0.5%)
11	K	0.45	0/1681	0.95	5/2274 (0.2%)
11	Y	0.46	0/1681	0.95	4/2274 (0.2%)
12	L	0.44	0/1795	1.04	13/2420 (0.5%)
12	Z	0.45	0/1795	1.03	11/2420 (0.5%)
13	M	0.46	0/1855	0.97	11/2514 (0.4%)
13	a	0.46	0/1855	0.97	10/2514 (0.4%)
14	N	0.49	0/1541	0.96	4/2087 (0.2%)
14	b	0.49	0/1541	0.97	4/2087 (0.2%)
15	c	1.51	0/6	0.93	0/7
15	d	1.55	0/6	0.92	0/7
15	e	1.57	0/6	0.96	0/7
15	f	1.33	0/6	0.93	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.45	0/50474	0.95	190/68220 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	35	ARG	N-CA-C	10.76	122.58	111.07
13	a	35	ARG	N-CA-C	10.74	122.56	111.07
11	K	189	GLY	N-CA-C	8.56	123.78	112.65
11	Y	189	GLY	N-CA-C	8.54	123.75	112.65
1	O	160	LYS	N-CA-C	-8.50	100.64	112.45
1	A	160	LYS	N-CA-C	-8.48	100.67	112.45
6	T	157	LYS	N-CA-C	-8.26	101.53	111.69
2	B	160	LYS	N-CA-C	-8.20	103.41	113.41
12	Z	103	PHE	CA-C-N	8.16	128.21	119.89
12	Z	103	PHE	C-N-CA	8.16	128.21	119.89
6	F	157	LYS	N-CA-C	-8.13	101.69	111.69
12	L	103	PHE	CA-C-N	7.82	127.86	119.89
12	L	103	PHE	C-N-CA	7.82	127.86	119.89
2	P	160	LYS	N-CA-C	-7.57	103.66	113.12
12	L	105	TYR	N-CA-C	-7.49	97.06	108.67
3	Q	103	THR	N-CA-C	-7.34	100.63	110.55
6	F	243	ILE	N-CA-C	-7.15	105.75	112.83
6	T	243	ILE	N-CA-C	-7.05	105.85	112.83
8	H	37	ILE	N-CA-C	-7.04	105.76	111.81
12	Z	105	TYR	N-CA-C	-6.98	97.86	108.67
3	C	103	THR	N-CA-C	-6.93	101.19	110.55
13	M	110	LEU	N-CA-C	-6.89	96.42	108.20
13	a	110	LEU	N-CA-C	-6.87	96.46	108.20
9	W	102	TYR	N-CA-C	-6.80	98.95	109.76
5	E	156	TYR	N-CA-C	-6.77	104.04	112.90
4	R	160	ASN	N-CA-C	-6.76	104.04	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	54	GLU	N-CA-C	-6.68	104.34	113.30
9	I	102	TYR	N-CA-C	-6.62	99.23	109.76
5	S	156	TYR	N-CA-C	-6.61	104.24	112.90
12	Z	146	ILE	N-CA-C	6.59	118.18	111.00
12	L	126	ASP	CA-C-N	-6.55	113.40	119.82
12	L	126	ASP	C-N-CA	-6.55	113.40	119.82
3	Q	158	SER	N-CA-C	-6.55	103.98	112.23
12	L	146	ILE	N-CA-C	6.54	118.12	111.00
1	O	75	TYR	N-CA-C	6.52	116.66	108.45
7	G	11	SER	N-CA-C	-6.47	101.93	110.40
5	E	54	GLU	N-CA-C	-6.44	104.67	113.30
4	D	160	ASN	N-CA-C	-6.43	104.48	112.90
4	R	168	SER	N-CA-C	6.43	117.97	110.97
8	V	37	ILE	N-CA-C	-6.42	106.29	111.81
4	D	168	SER	N-CA-C	6.42	117.94	111.07
12	Z	174	TYR	N-CA-C	6.38	119.50	110.50
7	U	11	SER	N-CA-C	-6.38	102.05	110.40
7	G	158	LYS	N-CA-C	-6.37	104.20	112.23
8	V	98	LEU	N-CA-C	6.36	119.90	109.72
8	H	98	LEU	N-CA-C	6.34	119.86	109.72
13	a	113	ALA	N-CA-C	-6.32	97.97	108.34
3	C	158	SER	N-CA-C	-6.31	104.28	112.23
6	F	131	SER	N-CA-C	-6.29	99.15	109.40
12	L	174	TYR	N-CA-C	6.29	119.36	110.50
13	M	106	LYS	N-CA-C	-6.29	105.19	112.92
7	U	158	LYS	N-CA-C	-6.28	104.32	112.23
12	Z	126	ASP	CA-C-N	-6.20	113.74	119.82
12	Z	126	ASP	C-N-CA	-6.20	113.74	119.82
2	B	135	ILE	N-CA-C	-6.19	98.71	107.75
3	C	131	THR	N-CA-C	6.18	119.09	109.52
2	P	135	ILE	N-CA-C	-6.17	98.75	107.75
2	P	70	ASP	N-CA-C	-6.16	105.80	113.38
13	a	106	LYS	N-CA-C	-6.16	105.35	112.92
1	A	126	GLY	N-CA-C	6.15	123.38	114.10
1	O	126	GLY	N-CA-C	6.13	123.35	114.10
7	U	223	LYS	N-CA-C	6.12	117.70	108.46
1	O	227	ILE	CA-C-N	6.10	125.58	119.24
1	O	227	ILE	C-N-CA	6.10	125.58	119.24
10	X	172	MET	CA-C-N	6.10	125.99	119.28
10	X	172	MET	C-N-CA	6.10	125.99	119.28
2	P	13	SER	N-CA-C	-6.09	103.12	110.13
6	T	131	SER	N-CA-C	-6.09	99.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	172	MET	CA-C-N	6.08	125.97	119.28
10	J	172	MET	C-N-CA	6.08	125.97	119.28
1	A	227	ILE	CA-C-N	6.04	125.53	119.24
1	A	227	ILE	C-N-CA	6.04	125.53	119.24
7	G	223	LYS	N-CA-C	6.04	117.58	108.46
12	L	128	VAL	N-CA-C	6.03	117.90	112.17
1	A	75	TYR	N-CA-C	6.01	116.03	108.45
2	P	107	VAL	N-CA-C	5.97	116.63	110.36
3	Q	21	ALA	N-CA-C	-5.97	104.78	111.28
13	M	113	ALA	N-CA-C	-5.96	98.57	108.34
10	X	128	LEU	CA-C-N	5.95	125.34	118.85
10	X	128	LEU	C-N-CA	5.95	125.34	118.85
13	a	7	THR	N-CA-C	5.93	118.88	109.50
10	X	129	PRO	N-CA-C	-5.91	105.48	113.40
2	B	70	ASP	N-CA-C	-5.90	106.13	113.38
13	M	7	THR	N-CA-C	5.88	118.79	109.50
9	W	67	ARG	N-CA-C	-5.87	104.79	111.07
1	A	100	ILE	CB-CA-C	-5.87	105.86	111.44
13	M	211	ASN	N-CA-C	5.85	119.63	111.90
4	R	127	SER	N-CA-C	5.85	118.44	111.71
10	X	28	LEU	N-CA-C	5.85	117.73	111.36
4	R	179	TRP	N-CA-C	5.83	119.03	109.76
12	Z	128	VAL	N-CA-C	5.81	117.81	111.77
4	R	53	SER	N-CA-C	5.80	119.89	112.34
11	Y	57	THR	N-CA-C	-5.80	105.04	111.36
11	Y	22	ALA	N-CA-C	-5.79	98.47	110.80
12	Z	104	PRO	N-CA-C	5.79	120.31	111.11
11	K	57	THR	N-CA-C	-5.78	105.06	111.36
8	H	38	SER	N-CA-C	-5.77	101.50	108.14
3	Q	131	THR	N-CA-C	5.77	118.46	109.52
5	E	97	VAL	N-CA-C	5.73	115.92	110.53
3	C	21	ALA	N-CA-C	-5.72	105.04	111.28
10	J	28	LEU	N-CA-C	5.72	117.59	111.36
4	D	74	THR	N-CA-C	5.70	118.26	111.71
13	M	17	ASP	N-CA-C	5.68	118.24	111.71
11	K	22	ALA	N-CA-C	-5.66	98.74	110.80
13	a	17	ASP	N-CA-C	5.65	118.21	111.71
4	D	179	TRP	N-CA-C	5.65	118.74	109.76
14	N	122	LEU	CA-C-N	5.62	124.98	118.85
14	N	122	LEU	C-N-CA	5.62	124.98	118.85
3	Q	65	ILE	N-CA-C	-5.61	105.63	111.58
13	a	211	ASN	N-CA-C	5.61	119.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	205	ALA	N-CA-C	-5.61	105.32	111.82
9	I	67	ARG	N-CA-C	-5.60	105.08	111.07
4	D	127	SER	N-CA-C	5.60	118.15	111.71
2	B	107	VAL	N-CA-C	5.59	116.99	110.62
13	M	39	VAL	N-CA-C	5.57	115.82	107.51
5	S	97	VAL	N-CA-C	5.57	115.77	110.53
4	D	126	MET	N-CA-C	-5.57	98.94	110.80
9	W	127	GLY	N-CA-C	5.57	123.00	115.32
6	F	67	ASP	CB-CA-C	-5.55	110.19	116.63
12	L	104	PRO	N-CA-C	5.53	119.91	111.11
10	X	195	PHE	N-CA-C	-5.51	106.46	114.12
1	A	63	LYS	N-CA-C	-5.50	106.61	113.38
9	I	153	TYR	N-CA-C	5.50	118.42	110.28
3	C	205	ALA	N-CA-C	-5.47	105.47	111.82
14	N	17	ASP	N-CA-C	-5.46	101.89	110.36
10	J	195	PHE	N-CA-C	-5.44	106.55	114.12
8	V	38	SER	N-CA-C	-5.43	101.89	108.14
4	R	225	ASN	N-CA-C	5.42	117.62	111.11
4	D	53	SER	N-CA-C	5.42	119.39	112.34
2	B	187	ASP	N-CA-C	-5.42	105.29	111.14
2	P	187	ASP	N-CA-C	-5.41	105.29	111.14
9	I	127	GLY	N-CA-C	5.40	122.78	115.32
14	N	128	GLY	N-CA-C	-5.40	106.82	111.95
1	O	63	LYS	N-CA-C	-5.40	106.86	113.50
1	O	100	ILE	CB-CA-C	-5.39	106.32	111.44
13	M	187	ARG	N-CA-C	5.39	120.52	113.30
9	I	189	ILE	N-CA-C	5.37	115.69	108.17
4	R	126	MET	N-CA-C	-5.37	99.35	110.80
10	J	128	LEU	N-CA-C	5.36	116.91	108.55
6	T	67	ASP	CB-CA-C	-5.36	110.41	116.63
4	R	74	THR	N-CA-C	5.35	117.86	111.71
9	W	153	TYR	N-CA-C	5.34	118.19	110.28
3	Q	186	VAL	N-CA-C	-5.34	104.42	111.09
4	D	225	ASN	N-CA-C	5.32	117.50	111.11
5	E	198	GLN	N-CA-C	-5.27	106.36	112.89
10	J	180	ILE	N-CA-C	-5.26	100.75	108.11
8	H	25	ILE	N-CA-C	5.25	115.51	108.17
9	I	101	PRO	N-CA-C	5.24	119.47	111.34
14	b	122	LEU	CA-C-N	5.24	124.56	118.85
14	b	122	LEU	C-N-CA	5.24	124.56	118.85
10	J	149	ARG	CA-C-N	5.23	126.37	119.84
10	J	149	ARG	C-N-CA	5.23	126.37	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	165	ASN	N-CA-C	5.21	119.36	112.89
2	B	13	SER	N-CA-C	-5.21	103.37	110.36
13	M	53	ILE	N-CA-C	5.21	115.99	108.48
10	X	147	HIS	N-CA-C	5.21	119.48	113.18
9	W	152	LEU	N-CA-C	5.20	117.69	111.71
13	a	39	VAL	N-CA-C	5.20	115.25	107.51
11	K	108	GLU	N-CA-C	5.20	119.75	113.41
3	C	186	VAL	N-CA-C	-5.19	104.61	111.09
12	Z	125	PHE	N-CA-C	5.17	117.67	109.50
14	b	128	GLY	N-CA-C	-5.16	107.05	111.95
11	Y	108	GLU	N-CA-C	5.15	119.70	113.41
3	C	65	ILE	N-CA-C	-5.15	106.12	111.58
12	L	125	PHE	N-CA-C	5.14	117.94	109.72
13	a	187	ARG	N-CA-C	5.14	120.40	113.72
14	b	17	ASP	N-CA-C	-5.14	101.90	109.86
13	M	104	ARG	N-CA-C	-5.13	105.87	111.82
4	D	201	GLU	N-CA-C	-5.12	105.59	111.07
12	L	30	ILE	N-CA-C	5.11	116.22	108.96
12	Z	32	ASP	CB-CA-C	-5.11	110.28	117.23
3	Q	170	ARG	N-CA-C	-5.10	105.81	111.36
8	V	165	ASN	N-CA-C	5.10	119.21	112.89
7	U	8	THR	N-CA-C	5.09	117.26	109.62
13	a	104	ARG	N-CA-C	-5.09	105.91	111.82
5	E	223	ILE	N-CA-C	5.09	115.30	108.17
6	T	151	GLY	N-CA-C	-5.09	108.31	114.92
10	X	180	ILE	N-CA-C	-5.08	101.00	108.11
5	S	149	SER	N-CA-C	-5.07	106.93	113.01
7	G	8	THR	N-CA-C	5.05	117.20	109.62
5	S	198	GLN	N-CA-C	-5.05	106.38	112.54
11	K	133	GLN	N-CA-C	5.05	117.17	111.11
7	U	178	LYS	N-CA-C	-5.04	105.91	111.71
5	S	223	ILE	N-CA-C	5.03	115.21	108.17
10	J	147	HIS	N-CA-C	5.02	119.26	113.18
12	L	133	ARG	N-CA-C	-5.02	101.52	109.96
10	X	171	ARG	N-CA-C	5.02	119.46	113.23
12	L	121	ALA	N-CA-C	5.01	116.99	109.23
6	T	34	ILE	N-CA-C	5.00	115.39	108.23
6	F	8	ASN	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	174	TYR	Sidechain
12	Z	174	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	72	0
1	O	1915	0	1929	67	0
2	B	1905	0	1904	94	0
2	P	1905	0	1904	93	0
3	C	1891	0	1903	82	0
3	Q	1891	0	1903	86	0
4	D	1862	0	1839	72	0
4	R	1862	0	1839	81	0
5	E	1795	0	1800	101	0
5	S	1795	0	1800	101	0
6	F	1897	0	1889	86	0
6	T	1897	0	1889	86	0
7	G	1921	0	1913	77	0
7	U	1921	0	1913	78	0
8	H	1685	0	1687	49	0
8	V	1685	0	1687	52	0
9	I	1581	0	1574	57	0
9	W	1581	0	1574	51	0
10	J	1585	0	1590	68	0
10	X	1585	0	1590	71	0
11	K	1644	0	1594	52	0
11	Y	1644	0	1594	53	0
12	L	1757	0	1711	69	0
12	Z	1757	0	1711	71	0
13	M	1824	0	1832	62	0
13	a	1824	0	1832	64	0
14	N	1512	0	1481	48	0
14	b	1512	0	1481	54	0
15	c	38	0	36	2	0
15	d	38	0	36	0	0
15	e	38	0	36	2	0
15	f	38	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	55	0	0	5	0
16	B	37	0	0	4	0
16	C	41	0	0	3	0
16	D	40	0	0	5	0
16	E	23	0	0	6	0
16	F	46	0	0	3	0
16	G	59	0	0	2	0
16	H	53	0	0	4	0
16	I	68	0	0	6	0
16	J	51	0	0	2	0
16	K	43	0	0	2	0
16	L	58	0	0	2	0
16	M	71	0	0	5	0
16	N	58	0	0	3	0
16	O	33	0	0	1	0
16	P	27	0	0	3	0
16	Q	26	0	0	3	0
16	R	28	0	0	5	0
16	S	21	0	0	2	0
16	T	38	0	0	6	0
16	U	62	0	0	2	0
16	V	47	0	0	3	0
16	W	57	0	0	2	0
16	X	47	0	0	3	0
16	Y	41	0	0	4	0
16	Z	55	0	0	2	0
16	a	74	0	0	5	0
16	b	60	0	0	4	0
16	f	1	0	0	0	0
All	All	51020	0	49436	1807	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.04	1.19
11:K:107:LYS:H	11:K:107:LYS:HD2	1.04	1.16
12:L:52:MET:HB2	12:L:111:ILE:HG22	1.34	1.10
10:J:174:MET:HE3	10:X:174:MET:HE3	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG2	2:B:55:LEU:HD21	1.15	1.08
12:Z:52:MET:HB2	12:Z:111:ILE:HG22	1.32	1.06
2:P:200:THR:HG22	2:P:202:SER:H	1.17	1.05
2:B:200:THR:HG22	2:B:202:SER:H	1.18	1.04
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.40	1.03
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.40	1.02
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.23	1.01
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.25	1.00
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.27	0.99
10:J:1:MET:HG2	10:J:2:ASP:H	1.30	0.97
10:X:1:MET:HG2	10:X:2:ASP:H	1.30	0.96
9:I:14:MET:HE3	9:I:166:ILE:HG12	1.45	0.96
1:O:176:GLU:HG2	2:P:55:LEU:HD21	1.47	0.95
2:P:69:ASN:ND2	2:P:70:ASP:H	1.65	0.95
13:M:179:ASN:HD22	13:M:182:ARG:HH11	0.98	0.95
7:G:92:ALA:HA	7:G:103:MET:HE2	1.49	0.94
9:W:14:MET:HE3	9:W:166:ILE:HG12	1.45	0.94
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.32	0.94
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.31	0.93
5:S:178:PHE:HA	5:S:181:ILE:HG12	1.51	0.93
13:a:179:ASN:HD22	13:a:182:ARG:HH11	0.98	0.93
2:B:69:ASN:ND2	2:B:70:ASP:H	1.66	0.92
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.34	0.90
2:P:49:ARG:HH22	2:P:61:SER:HB3	1.36	0.90
3:Q:60:SER:HB2	16:Q:303:HOH:O	1.71	0.89
2:B:49:ARG:HH22	2:B:61:SER:HB3	1.36	0.89
7:U:92:ALA:HA	7:U:103:MET:HE2	1.52	0.89
5:E:178:PHE:HA	5:E:181:ILE:HG12	1.52	0.89
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.38	0.89
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.40	0.87
11:Y:107:LYS:HD2	11:Y:107:LYS:N	1.89	0.87
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.39	0.87
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.40	0.86
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.40	0.85
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.41	0.85
1:O:128:ARG:HH21	7:U:120:THR:CG2	1.90	0.85
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.58	0.84
3:C:185:THR:HG22	3:C:187:GLU:H	1.43	0.84
11:K:107:LYS:HD2	11:K:107:LYS:N	1.90	0.84
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.23	0.84
5:E:205:LEU:HA	5:E:209:ASN:ND2	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.40	0.84
5:S:205:LEU:HA	5:S:209:ASN:ND2	1.92	0.83
13:a:119:VAL:HG23	13:a:200:ILE:HG22	1.60	0.83
7:G:55:LEU:O	7:G:57:PRO:HD3	1.79	0.83
1:A:176:GLU:CG	2:B:55:LEU:HD21	2.06	0.82
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.45	0.82
10:X:162:LYS:O	10:X:166:GLN:HG3	1.79	0.82
13:M:48:ASN:H	13:M:48:ASN:HD22	1.26	0.82
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.61	0.82
5:E:205:LEU:HD23	5:E:205:LEU:H	1.45	0.81
13:a:161:ARG:HH11	13:a:161:ARG:HG3	1.45	0.81
1:O:12:PHE:H	2:P:20:GLN:HE22	1.24	0.81
5:S:205:LEU:H	5:S:205:LEU:HD23	1.45	0.81
10:J:162:LYS:O	10:J:166:GLN:HG3	1.80	0.81
7:U:55:LEU:O	7:U:57:PRO:HD3	1.81	0.81
1:A:128:ARG:HH21	7:G:120:THR:CG2	1.94	0.81
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.45	0.81
2:B:223:GLU:HG2	2:B:224:VAL:H	1.44	0.81
5:E:162:ALA:HB3	16:E:320:HOH:O	1.80	0.80
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.46	0.80
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.46	0.80
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.61	0.80
3:Q:233:GLN:O	3:Q:237:GLU:HG2	1.82	0.80
13:a:48:ASN:HD22	13:a:48:ASN:H	1.28	0.80
2:P:223:GLU:HG2	2:P:224:VAL:H	1.46	0.80
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.64	0.79
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.63	0.79
3:C:233:GLN:O	3:C:237:GLU:HG2	1.83	0.79
10:J:174:MET:HE3	10:X:174:MET:CE	2.12	0.79
10:X:33:ASP:OD2	10:X:35:THR:HG22	1.83	0.79
1:A:29:LYS:HE2	1:A:29:LYS:HA	1.65	0.78
7:G:202:ILE:HG23	7:G:207:THR:O	1.82	0.78
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.66	0.78
2:B:12:PHE:H	3:C:17:GLN:HE22	1.28	0.78
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.48	0.78
7:U:221:LYS:HE3	7:U:221:LYS:HA	1.65	0.78
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.14	0.78
4:D:200:MET:HE1	4:D:208:ASN:ND2	1.99	0.78
11:Y:107:LYS:H	11:Y:107:LYS:CD	1.88	0.78
7:G:221:LYS:HA	7:G:221:LYS:HE3	1.66	0.78
12:L:195:HIS:HD2	12:L:197:GLN:H	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.65	0.78
1:O:122:THR:CG2	2:P:128:ARG:HH21	1.96	0.78
1:A:239:THR:OG1	1:A:242:GLU:HG3	1.85	0.77
1:O:29:LYS:HE2	1:O:29:LYS:HA	1.66	0.77
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.65	0.77
2:B:200:THR:HG22	2:B:202:SER:N	1.99	0.77
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.20	0.77
10:J:174:MET:CE	10:X:174:MET:HE3	2.11	0.76
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.68	0.76
13:a:179:ASN:HD22	13:a:182:ARG:NH1	1.81	0.76
6:F:31:THR:HG21	6:F:47:GLU:O	1.84	0.76
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.66	0.76
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.66	0.76
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.21	0.76
1:A:122:THR:CG2	2:B:128:ARG:HH21	1.99	0.76
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.00	0.76
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.30	0.75
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.67	0.75
2:P:200:THR:HG22	2:P:202:SER:N	1.99	0.75
7:U:202:ILE:HG23	7:U:207:THR:O	1.85	0.75
1:A:12:PHE:H	2:B:20:GLN:HE22	1.31	0.75
6:T:31:THR:HG21	6:T:47:GLU:O	1.84	0.75
10:X:149:ARG:O	10:X:152:MET:HG3	1.87	0.75
10:J:33:ASP:OD2	10:J:35:THR:HG22	1.85	0.75
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.17	0.75
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.68	0.75
10:J:149:ARG:O	10:J:152:MET:HG3	1.87	0.75
1:O:239:THR:OG1	1:O:242:GLU:HG3	1.86	0.75
3:Q:95:ARG:NH1	3:Q:101:PRO:HB3	2.01	0.75
6:F:65:VAL:HG12	16:F:308:HOH:O	1.86	0.74
11:K:64:ARG:HD2	16:K:330:HOH:O	1.87	0.74
3:C:95:ARG:NH1	3:C:101:PRO:HB3	2.03	0.74
8:V:52:THR:O	8:V:56:THR:HB	1.87	0.74
5:S:197:SER:HA	5:S:200:LEU:HG	1.69	0.74
9:I:176:ARG:NH2	12:Z:147:MET:HE3	2.02	0.74
12:L:17:GLY:HA3	12:L:20:PHE:CE2	2.23	0.74
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.35	0.74
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.67	0.74
5:S:136:TYR:CE2	5:S:217:LYS:HA	2.23	0.74
12:Z:17:GLY:HA3	12:Z:20:PHE:CE2	2.22	0.74
7:G:117:GLN:O	7:G:120:THR:HB	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:122:GLU:HG2	4:R:123:GLU:H	1.51	0.74
4:R:200:MET:HE1	4:R:208:ASN:ND2	2.03	0.73
13:a:89:PRO:HD2	13:a:120:GLN:OE1	1.87	0.73
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.71	0.73
7:U:117:GLN:O	7:U:120:THR:HB	1.89	0.73
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.33	0.73
1:A:178:ARG:NH1	1:A:178:ARG:HB3	2.04	0.73
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.02	0.73
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.23	0.73
13:M:179:ASN:HD22	13:M:182:ARG:NH1	1.81	0.73
1:A:17:LYS:HE3	1:A:22:ASP:OD1	1.89	0.73
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.71	0.73
1:O:178:ARG:HB3	1:O:178:ARG:NH1	2.03	0.73
8:H:135:MET:HE3	13:a:187:ARG:NH2	2.03	0.73
13:M:89:PRO:HD2	13:M:120:GLN:OE1	1.88	0.73
8:H:52:THR:O	8:H:56:THR:HB	1.87	0.73
3:Q:64:LYS:HE3	3:Q:219:ILE:HD12	1.70	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.36	0.72
4:D:122:GLU:HG2	4:D:123:GLU:H	1.52	0.72
2:P:69:ASN:ND2	2:P:70:ASP:N	2.37	0.72
2:B:48:GLU:OE2	2:B:200:THR:HG23	1.89	0.72
9:W:35:VAL:HG13	16:X:224:HOH:O	1.89	0.72
6:T:65:VAL:HG12	16:T:324:HOH:O	1.90	0.72
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.73	0.71
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.72	0.71
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.38	0.71
5:S:81:ARG:HH11	5:S:81:ARG:HG3	1.54	0.71
12:L:147:MET:HE3	9:W:176:ARG:NH2	2.05	0.71
3:C:64:LYS:HE3	3:C:219:ILE:HD12	1.72	0.71
5:E:81:ARG:HH11	5:E:81:ARG:HG3	1.55	0.71
5:E:197:SER:HA	5:E:200:LEU:HG	1.71	0.71
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.53	0.71
6:T:143:HIS:HD2	16:T:301:HOH:O	1.72	0.71
11:K:12:ILE:HB	11:K:180:VAL:HB	1.72	0.71
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.27	0.70
1:A:187:ASP:O	1:A:191:ILE:HG12	1.91	0.70
2:P:48:GLU:OE2	2:P:200:THR:HG23	1.89	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.73	0.70
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.27	0.70
9:I:148:MET:HE3	9:I:152:LEU:HD11	1.73	0.70
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:187:ASP:O	1:O:191:ILE:HG12	1.92	0.70
2:B:69:ASN:ND2	2:B:70:ASP:N	2.39	0.70
6:T:75:SER:HA	16:T:334:HOH:O	1.91	0.70
8:V:195:VAL:HG23	16:V:321:HOH:O	1.92	0.69
2:P:141:ASP:OD2	10:X:110:LYS:HE2	1.91	0.69
4:D:176:LEU:HD22	5:E:55:LEU:HD11	1.75	0.69
3:Q:213:VAL:HG23	3:Q:219:ILE:HG12	1.75	0.69
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.74	0.69
4:D:60:VAL:HG21	4:D:81:ILE:HD13	1.74	0.69
4:R:60:VAL:HG21	4:R:81:ILE:HD13	1.74	0.69
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.72	0.69
3:C:213:VAL:HG23	3:C:219:ILE:HG12	1.75	0.69
2:P:69:ASN:HD22	2:P:70:ASP:N	1.90	0.69
4:R:64:ARG:HG3	16:R:328:HOH:O	1.92	0.69
1:O:83:ARG:HE	7:U:114:ASN:ND2	1.90	0.68
9:W:148:MET:HE3	9:W:152:LEU:HD11	1.75	0.68
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.29	0.68
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.75	0.68
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.06	0.68
4:R:191:LEU:O	4:R:195:ILE:HG12	1.93	0.68
13:a:179:ASN:ND2	13:a:182:ARG:HH11	1.83	0.68
2:B:69:ASN:HD22	2:B:70:ASP:N	1.92	0.68
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.74	0.68
8:H:135:MET:HE3	13:a:187:ARG:CZ	2.22	0.68
13:M:187:ARG:NH2	8:V:135:MET:HE3	2.09	0.68
12:L:126:ASP:HB2	12:L:130:SER:H	1.57	0.68
1:O:178:ARG:HB3	1:O:178:ARG:HH11	1.59	0.67
12:Z:126:ASP:HB2	12:Z:130:SER:H	1.59	0.67
1:A:178:ARG:HB3	1:A:178:ARG:HH11	1.60	0.67
1:O:17:LYS:HE3	1:O:22:ASP:OD1	1.95	0.67
1:O:82:TYR:O	1:O:86:VAL:HG23	1.95	0.67
2:P:122:THR:CG2	3:Q:125:ARG:HH21	2.07	0.67
5:S:12:PHE:HB2	6:T:19:GLN:NE2	2.07	0.67
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.43	0.67
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.58	0.67
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.60	0.67
2:P:85:ILE:O	2:P:89:THR:HG23	1.95	0.67
4:R:185:LEU:O	4:R:189:GLU:HG3	1.95	0.67
5:S:181:ILE:CG2	5:S:187:GLU:HB2	2.25	0.67
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.43	0.67
5:E:172:GLU:OE1	6:F:52:SER:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:45:ARG:O	4:R:45:ARG:HG2	1.95	0.67
13:a:27:LEU:HB2	13:a:192:SER:HB2	1.76	0.67
11:K:196:LEU:O	11:K:200:VAL:HG23	1.95	0.66
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.05	0.66
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.76	0.66
2:P:184:LYS:HD3	2:P:185:VAL:N	2.10	0.66
5:S:99:ASN:HB2	13:a:94:GLU:HG2	1.77	0.66
5:E:181:ILE:CG2	5:E:187:GLU:HB2	2.25	0.66
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.61	0.66
4:D:191:LEU:O	4:D:195:ILE:HG12	1.95	0.66
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.30	0.66
13:M:179:ASN:ND2	13:M:182:ARG:HH11	1.83	0.66
7:U:83:ASN:HD22	7:U:83:ASN:C	2.02	0.66
2:B:184:LYS:HD3	2:B:185:VAL:N	2.10	0.66
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.61	0.66
11:K:107:LYS:H	11:K:107:LYS:CD	1.88	0.66
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.31	0.66
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.77	0.66
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.78	0.66
11:Y:196:LEU:O	11:Y:200:VAL:HG23	1.95	0.66
1:A:82:TYR:O	1:A:86:VAL:HG23	1.96	0.66
7:G:92:ALA:CA	7:G:103:MET:HE2	2.23	0.65
2:P:119:GLN:O	2:P:122:THR:HB	1.95	0.65
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.78	0.65
3:C:185:THR:HB	3:C:188:GLU:HG2	1.79	0.65
12:L:30:ILE:C	12:L:30:ILE:HD12	2.22	0.65
2:B:119:GLN:O	2:B:122:THR:HB	1.97	0.65
13:M:187:ARG:CZ	8:V:135:MET:HE3	2.27	0.65
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.78	0.65
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.62	0.65
2:B:85:ILE:O	2:B:89:THR:HG23	1.97	0.65
8:H:81:GLN:O	8:H:85:GLN:HG3	1.95	0.65
12:L:100:LYS:HE3	12:L:103:PHE:O	1.96	0.65
2:B:141:ASP:OD2	10:J:110:LYS:HE2	1.98	0.64
7:G:73:VAL:CG1	7:G:133:THR:HB	2.27	0.64
1:A:83:ARG:HE	7:G:114:ASN:ND2	1.95	0.64
1:A:119:GLN:O	1:A:122:THR:HB	1.97	0.64
13:a:16:TYR:CE2	13:a:170:VAL:HG22	2.32	0.64
12:L:206:ILE:HD12	12:L:206:ILE:N	2.13	0.64
12:Z:206:ILE:N	12:Z:206:ILE:HD12	2.13	0.64
12:Z:52:MET:CB	12:Z:111:ILE:HG22	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:100:LYS:HE3	12:Z:103:PHE:O	1.96	0.64
3:C:51:LYS:O	3:C:52:LEU:HB2	1.97	0.64
8:V:81:GLN:O	8:V:85:GLN:HG3	1.97	0.64
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.78	0.64
2:B:148:TYR:CZ	3:C:57:ILE:HG13	2.33	0.64
5:E:178:PHE:HA	5:E:181:ILE:CG1	2.27	0.64
4:R:16:VAL:O	4:R:19:SER:HB3	1.98	0.64
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.79	0.64
9:I:97:ARG:HD2	16:I:364:HOH:O	1.98	0.64
5:S:189:ILE:HG23	5:S:212:ILE:HG21	1.80	0.64
7:U:92:ALA:CA	7:U:103:MET:HE2	2.25	0.64
8:V:218:VAL:HB	9:W:194:VAL:HB	1.80	0.64
1:O:66:LEU:HD23	1:O:66:LEU:C	2.24	0.63
5:S:178:PHE:HA	5:S:181:ILE:CG1	2.27	0.63
11:Y:99:THR:HG22	11:Y:115:VAL:O	1.98	0.63
4:D:185:LEU:O	4:D:189:GLU:HG3	1.99	0.63
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.28	0.63
12:Z:30:ILE:C	12:Z:30:ILE:HD12	2.23	0.63
2:B:55:LEU:N	2:B:55:LEU:HD22	2.13	0.63
7:U:73:VAL:CG1	7:U:133:THR:HB	2.28	0.63
5:S:189:ILE:O	5:S:193:VAL:HG23	1.97	0.63
10:X:1:MET:CG	10:X:2:ASP:H	2.09	0.63
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.79	0.63
10:X:1:MET:HG2	10:X:2:ASP:N	2.08	0.63
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.28	0.63
1:O:119:GLN:O	1:O:122:THR:HB	1.98	0.63
5:S:172:GLU:OE1	6:T:52:SER:HB2	1.99	0.63
5:S:179:ILE:O	5:S:179:ILE:HD13	1.98	0.63
4:D:16:VAL:O	4:D:19:SER:HB3	1.98	0.63
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.79	0.63
14:b:112:THR:HG22	14:b:120:HIS:HB2	1.80	0.63
5:E:189:ILE:O	5:E:193:VAL:HG23	1.99	0.63
10:J:158:LEU:HD13	10:J:198:GLN:HE22	1.64	0.63
12:L:22:VAL:HG12	12:L:206:ILE:HG13	1.80	0.63
12:L:103:PHE:N	12:L:104:PRO:HD3	2.14	0.63
9:W:171:LEU:HD11	9:W:201:MET:HB3	1.81	0.63
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.80	0.63
1:A:66:LEU:C	1:A:66:LEU:HD23	2.23	0.63
12:Z:103:PHE:N	12:Z:104:PRO:HD3	2.13	0.63
5:E:179:ILE:O	5:E:179:ILE:HD13	1.99	0.62
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:167:LEU:HD22	12:Z:196:ILE:O	1.99	0.62
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.98	0.62
4:D:45:ARG:O	4:D:45:ARG:HG2	1.98	0.62
10:J:153:THR:OG1	10:J:156:GLU:HG3	1.99	0.62
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.82	0.62
7:G:73:VAL:HG12	7:G:133:THR:HB	1.82	0.62
2:P:99:LYS:NZ	10:X:86:GLN:HE22	1.98	0.62
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.81	0.62
4:D:6:THR:HG23	5:E:20:GLN:NE2	2.15	0.62
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	1.82	0.62
7:G:83:ASN:C	7:G:83:ASN:HD22	2.07	0.62
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.81	0.62
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.81	0.62
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.81	0.62
2:P:55:LEU:HD22	2:P:55:LEU:N	2.15	0.62
4:R:193:LEU:HD22	4:R:211:LEU:HD11	1.80	0.62
10:X:158:LEU:HD13	10:X:198:GLN:HE22	1.63	0.62
1:A:169:VAL:HG23	16:A:317:HOH:O	1.99	0.62
9:I:171:LEU:HD11	9:I:201:MET:HB3	1.82	0.62
5:S:154:GLU:OE2	6:T:59:LYS:HD2	2.00	0.62
10:X:53:THR:HG23	10:X:54:VAL:N	2.15	0.62
6:F:66:VAL:HB	6:F:70:ILE:HB	1.82	0.62
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.81	0.62
2:P:93:HIS:HB2	16:P:304:HOH:O	2.00	0.62
5:E:189:ILE:HG23	5:E:212:ILE:HG21	1.81	0.61
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.30	0.61
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.82	0.61
4:D:241:ALA:O	4:D:242:GLU:HB2	2.00	0.61
10:J:1:MET:HG2	10:J:2:ASP:N	2.08	0.61
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.82	0.61
5:S:207:VAL:HG13	5:S:208:ASP:N	2.15	0.61
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.81	0.61
11:K:99:THR:HG22	11:K:115:VAL:O	2.01	0.61
5:S:200:LEU:O	5:S:201:ARG:HB2	2.00	0.61
13:a:174:GLU:O	13:a:178:VAL:HG23	2.00	0.61
5:E:77:ALA:HB3	5:E:78:PRO:HD3	1.82	0.61
5:E:205:LEU:H	5:E:205:LEU:CD2	2.14	0.61
12:L:52:MET:CB	12:L:111:ILE:HG22	2.19	0.61
10:J:117:TYR:CE1	10:J:127:GLU:HG3	2.35	0.61
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.81	0.61
5:S:77:ALA:HB3	5:S:78:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:C	1:A:250:LEU:H	2.09	0.61
10:J:53:THR:HG23	10:J:54:VAL:N	2.13	0.61
2:P:244:THR:OXT	2:P:244:THR:HG22	2.00	0.61
4:R:89:VAL:HG21	11:Y:65:LEU:HD22	1.83	0.61
4:R:241:ALA:O	4:R:242:GLU:HB2	1.99	0.61
5:S:205:LEU:H	5:S:205:LEU:CD2	2.14	0.61
6:T:66:VAL:HB	6:T:70:ILE:HB	1.82	0.61
1:A:30:GLN:HE21	1:A:30:GLN:HA	1.65	0.61
5:E:207:VAL:HG13	5:E:208:ASP:N	2.16	0.61
1:O:158:PRO:O	2:P:56:LEU:HD12	2.01	0.61
1:O:30:GLN:HA	1:O:30:GLN:HE21	1.65	0.61
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.81	0.61
7:U:73:VAL:HG12	7:U:133:THR:HB	1.81	0.61
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.83	0.60
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.31	0.60
4:R:113:LEU:HB2	16:R:317:HOH:O	2.01	0.60
10:X:117:TYR:CE1	10:X:127:GLU:HG3	2.36	0.60
5:E:55:LEU:N	5:E:55:LEU:HD12	2.16	0.60
4:D:89:VAL:HG11	11:K:65:LEU:CD2	2.32	0.60
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.82	0.60
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.84	0.60
1:O:248:GLU:C	1:O:250:LEU:H	2.09	0.60
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.84	0.60
4:R:89:VAL:HG11	11:Y:65:LEU:CD2	2.32	0.60
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.81	0.60
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.83	0.60
14:b:175:MET:HE3	14:b:188:PHE:CE2	2.36	0.60
1:A:172:LYS:O	1:A:176:GLU:HG3	2.02	0.60
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.82	0.60
5:S:55:LEU:N	5:S:55:LEU:HD12	2.17	0.60
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.30	0.60
2:B:220:ASN:O	2:B:221:ASP:HB2	2.01	0.60
14:N:175:MET:HE3	14:N:188:PHE:CE2	2.35	0.60
5:E:200:LEU:O	5:E:201:ARG:HB2	2.01	0.60
14:N:114:PRO:HD2	14:N:118:SER:O	2.02	0.60
5:S:127:TYR:O	5:S:148:PRO:HB3	2.02	0.60
7:U:241:GLU:O	7:U:242:GLN:HB2	2.02	0.60
2:B:223:GLU:HG2	2:B:224:VAL:N	2.17	0.59
3:C:35:LYS:HD3	3:C:158:SER:HA	1.84	0.59
4:D:193:LEU:HD22	4:D:211:LEU:HD11	1.83	0.59
5:E:205:LEU:HD23	5:E:205:LEU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:31:VAL:HA	12:Z:132:GLU:OE2	2.02	0.59
8:H:34:LEU:HB2	16:H:326:HOH:O	2.02	0.59
8:H:195:VAL:HA	16:H:348:HOH:O	2.01	0.59
7:U:169:ILE:HD12	7:U:201:MET:CE	2.32	0.59
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.32	0.59
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.01	0.59
10:X:153:THR:OG1	10:X:156:GLU:HG3	2.03	0.59
16:B:319:HOH:O	3:C:27:ARG:HD2	2.02	0.59
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.83	0.59
2:P:99:LYS:HZ2	10:X:86:GLN:HE22	1.49	0.59
3:Q:35:LYS:HD3	3:Q:158:SER:HA	1.85	0.59
14:b:112:THR:CG2	14:b:120:HIS:HB2	2.33	0.59
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.84	0.59
4:D:104:LEU:C	4:D:104:LEU:HD13	2.27	0.59
13:M:174:GLU:O	13:M:178:VAL:HG23	2.03	0.59
12:Z:14:GLY:O	12:Z:136:CYS:HA	2.02	0.59
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.84	0.59
14:b:66:TYR:CD2	14:b:73:PRO:HB3	2.37	0.59
4:D:89:VAL:HG21	11:K:65:LEU:HD22	1.83	0.59
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.84	0.59
5:E:45:LEU:HG	5:E:134:ILE:HD13	1.85	0.59
7:U:167:GLN:NE2	7:U:171:THR:HG23	2.18	0.59
14:b:105:LYS:HD3	14:b:105:LYS:C	2.28	0.59
2:B:244:THR:OXT	2:B:244:THR:HG22	2.03	0.59
7:G:167:GLN:NE2	7:G:171:THR:HG23	2.17	0.59
2:P:220:ASN:O	2:P:221:ASP:HB2	2.02	0.59
14:b:144:GLU:HG2	16:b:255:HOH:O	2.02	0.59
3:C:172:PHE:O	3:C:176:ASN:HB2	2.03	0.58
11:K:106:ARG:HD3	11:K:182:GLU:OE1	2.03	0.58
7:U:51:PRO:HG2	7:U:52:ASP:H	1.67	0.58
9:W:17:LYS:HD3	9:W:156:ASN:HD22	1.68	0.58
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.84	0.58
13:a:129:TYR:HE1	13:a:144:THR:HG22	1.68	0.58
6:F:105:ILE:HG21	6:F:143:HIS:HB2	1.85	0.58
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.85	0.58
12:Z:2:PHE:HB2	13:a:1:THR:HG23	1.85	0.58
1:O:172:LYS:O	1:O:176:GLU:HG3	2.03	0.58
12:Z:202:LEU:HB2	12:Z:219:LEU:HD11	1.85	0.58
3:C:34:VAL:HG12	3:C:159:ALA:HB1	1.85	0.58
11:Y:106:ARG:HD3	11:Y:182:GLU:OE1	2.03	0.58
7:G:169:ILE:HD12	7:G:201:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.39	0.58
3:Q:167:LYS:HB2	16:Q:313:HOH:O	2.02	0.58
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.84	0.58
9:I:123:PHE:CD2	9:I:123:PHE:N	2.72	0.58
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.32	0.58
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.85	0.58
6:T:105:ILE:HG21	6:T:143:HIS:HB2	1.85	0.58
7:G:241:GLU:O	7:G:242:GLN:HB2	2.03	0.58
12:L:2:PHE:HB2	13:M:1:THR:HG23	1.86	0.58
12:L:14:GLY:O	12:L:136:CYS:HA	2.03	0.58
9:W:50:LEU:CD2	9:W:52:ILE:HD11	2.34	0.58
1:A:204:PHE:CE1	1:A:209:ILE:HD11	2.39	0.58
13:M:49:THR:OG1	13:M:89:PRO:HG3	2.04	0.58
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.04	0.58
12:L:202:LEU:HB2	12:L:219:LEU:HD11	1.85	0.57
1:O:128:ARG:NH2	7:U:120:THR:HG22	2.12	0.57
3:Q:34:VAL:HG12	3:Q:159:ALA:HB1	1.86	0.57
16:E:319:HOH:O	12:L:73:LYS:HE3	2.04	0.57
7:G:39:LYS:HB2	7:G:187:GLU:O	2.03	0.57
7:G:189:SER:HB2	7:G:191:GLU:OE2	2.03	0.57
14:N:14:LEU:O	14:N:175:MET:HA	2.03	0.57
1:O:246:ARG:HG3	1:O:246:ARG:HH11	1.69	0.57
7:G:51:PRO:HG2	7:G:52:ASP:H	1.68	0.57
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.87	0.57
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.85	0.57
3:Q:51:LYS:HD2	3:Q:52:LEU:N	2.19	0.57
5:E:127:TYR:O	5:E:148:PRO:HB3	2.03	0.57
10:J:53:THR:CG2	10:J:54:VAL:N	2.66	0.57
11:K:31:VAL:HA	12:L:132:GLU:OE2	2.04	0.57
6:T:185:ALA:O	6:T:189:VAL:HG23	2.04	0.57
7:U:39:LYS:HB2	7:U:187:GLU:O	2.05	0.57
6:F:83:HIS:HD2	6:F:128:PHE:CE2	2.22	0.57
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.04	0.57
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.04	0.57
3:C:160:GLN:NE2	3:C:161:THR:H	2.02	0.57
6:F:32:THR:HG23	6:F:47:GLU:OE2	2.05	0.57
6:F:83:HIS:HD2	6:F:128:PHE:HE2	1.52	0.57
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.87	0.57
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.69	0.57
14:N:105:LYS:C	14:N:105:LYS:HD3	2.29	0.57
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:51:ASN:ND2	5:S:53:ASP:O	2.38	0.57
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.86	0.57
5:E:181:ILE:HG21	5:E:187:GLU:HB2	1.87	0.57
6:F:185:ALA:O	6:F:189:VAL:HG23	2.05	0.57
12:L:196:ILE:O	8:V:167:LEU:HD22	2.05	0.57
2:P:44:VAL:HG22	2:P:214:THR:HG22	1.85	0.57
7:U:103:MET:HE3	7:U:108:LEU:HB2	1.87	0.57
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.86	0.57
3:Q:155:SER:HB2	4:R:51:LEU:HD21	1.87	0.57
3:Q:172:PHE:O	3:Q:176:ASN:HB2	2.05	0.57
6:T:83:HIS:HD2	6:T:128:PHE:HE2	1.52	0.57
2:B:49:ARG:HH22	2:B:61:SER:CB	2.14	0.56
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.87	0.56
4:D:67:GLY:HA3	4:D:220:PHE:CD2	2.40	0.56
4:D:184:THR:OG1	4:D:187:GLU:HG3	2.05	0.56
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.87	0.56
3:Q:156:SER:HB2	16:Q:320:HOH:O	2.04	0.56
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.40	0.56
13:a:49:THR:OG1	13:a:89:PRO:HG3	2.05	0.56
14:b:14:LEU:O	14:b:175:MET:HA	2.05	0.56
9:I:50:LEU:CD2	9:I:52:ILE:HD11	2.35	0.56
9:I:202:ARG:HD3	16:I:365:HOH:O	2.05	0.56
14:N:114:PRO:HG2	16:N:206:HOH:O	2.05	0.56
1:O:3:ASP:OD2	1:O:5:TYR:HB2	2.05	0.56
5:S:45:LEU:HG	5:S:134:ILE:HD13	1.86	0.56
9:W:50:LEU:HG	9:W:52:ILE:HD11	1.87	0.56
4:D:186:LYS:O	4:D:190:LEU:HD23	2.05	0.56
5:E:154:GLU:OE2	6:F:59:LYS:HD2	2.05	0.56
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.87	0.56
1:O:59:GLU:H	1:O:59:GLU:CD	2.13	0.56
2:P:239:VAL:HG12	2:P:240:LYS:HD3	1.87	0.56
4:R:186:LYS:O	4:R:190:LEU:HD23	2.05	0.56
6:T:83:HIS:HD2	6:T:128:PHE:CE2	2.23	0.56
6:T:148:GLU:HB3	16:T:338:HOH:O	2.03	0.56
11:Y:147:ASP:O	11:Y:148:LEU:C	2.48	0.56
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.87	0.56
3:C:101:PRO:HG2	3:C:138:PRO:CG	2.36	0.56
3:C:186:VAL:O	3:C:190:VAL:HG23	2.04	0.56
5:E:226:GLY:O	5:E:229:VAL:HG22	2.05	0.56
6:F:186:ARG:HG3	6:F:186:ARG:HH11	1.71	0.56
13:M:19:GLY:HA3	13:M:200:ILE:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:57:GLU:HA	16:R:311:HOH:O	2.04	0.56
14:b:114:PRO:HD2	14:b:118:SER:O	2.05	0.56
3:C:51:LYS:HD2	3:C:52:LEU:N	2.21	0.56
6:F:169:LYS:O	6:F:173:GLU:HG3	2.06	0.56
13:M:119:VAL:CG2	13:M:200:ILE:HG22	2.32	0.56
3:Q:101:PRO:HG2	3:Q:138:PRO:CG	2.35	0.56
13:a:51:VAL:HG22	13:a:116:VAL:HG22	1.85	0.56
9:I:14:MET:CE	9:I:166:ILE:HG12	2.27	0.56
9:I:148:MET:HE2	9:I:172:ASN:HB2	1.88	0.56
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.88	0.56
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.87	0.56
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.41	0.56
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.41	0.56
2:P:119:GLN:NE2	16:P:311:HOH:O	2.39	0.56
3:Q:160:GLN:NE2	3:Q:161:THR:H	2.03	0.56
5:S:226:GLY:O	5:S:229:VAL:HG22	2.06	0.56
7:U:189:SER:HB2	7:U:191:GLU:OE2	2.05	0.56
6:F:220:THR:O	6:F:221:ASN:HB2	2.06	0.56
4:R:204:LEU:HD23	4:R:204:LEU:C	2.30	0.56
6:T:50:ILE:HG13	6:T:208:PHE:HA	1.88	0.56
14:b:105:LYS:HD3	14:b:105:LYS:O	2.05	0.56
2:B:217:LYS:O	2:B:218:GLY:C	2.48	0.56
12:L:3:ASN:HD22	12:L:4:PRO:CD	2.18	0.56
2:P:223:GLU:HG2	2:P:224:VAL:N	2.19	0.56
6:T:186:ARG:HH11	6:T:186:ARG:HG3	1.70	0.56
14:N:161:GLN:HE22	14:b:139:ASP:HB3	1.71	0.55
6:T:172:LEU:O	6:T:176:VAL:HG23	2.06	0.55
1:A:246:ARG:HH11	1:A:246:ARG:HG3	1.70	0.55
5:E:207:VAL:CG1	5:E:208:ASP:N	2.70	0.55
14:N:105:LYS:HD3	14:N:105:LYS:O	2.06	0.55
14:N:139:ASP:HB3	14:b:161:GLN:HE22	1.70	0.55
2:P:233:GLU:O	2:P:237:ILE:HG22	2.06	0.55
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.87	0.55
10:X:53:THR:CG2	10:X:54:VAL:N	2.69	0.55
9:I:50:LEU:HG	9:I:52:ILE:HD11	1.89	0.55
4:R:94:TYR:O	12:Z:91:ARG:HG3	2.05	0.55
10:X:149:ARG:HG2	10:X:149:ARG:HH11	1.71	0.55
13:a:168:THR:HA	16:a:322:HOH:O	2.04	0.55
8:H:218:VAL:HB	9:I:194:VAL:HB	1.89	0.55
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.89	0.55
9:W:154:GLU:HG3	9:W:157:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.87	0.55
13:a:48:ASN:HD22	13:a:48:ASN:N	1.94	0.55
1:A:90:ARG:NH1	16:A:309:HOH:O	2.32	0.55
2:B:233:GLU:O	2:B:237:ILE:HG22	2.06	0.55
7:G:75:ASN:HA	16:G:344:HOH:O	2.05	0.55
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.42	0.55
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.88	0.55
3:C:197:LEU:O	3:C:201:VAL:HG23	2.06	0.55
4:D:176:LEU:HD22	5:E:55:LEU:CD1	2.37	0.55
10:J:17:SER:HB2	16:J:210:HOH:O	2.06	0.55
14:N:161:GLN:NE2	14:b:136:GLY:HA2	2.09	0.55
2:P:180:LYS:HE2	2:P:182:ASP:OD1	2.07	0.55
2:P:217:LYS:O	2:P:218:GLY:C	2.49	0.55
4:R:104:LEU:C	4:R:104:LEU:HD13	2.32	0.55
13:a:19:GLY:HA3	13:a:200:ILE:O	2.06	0.55
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.88	0.55
5:S:205:LEU:HD23	5:S:205:LEU:N	2.17	0.55
5:S:207:VAL:CG1	5:S:208:ASP:N	2.69	0.55
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.06	0.55
6:T:169:LYS:O	6:T:173:GLU:HG3	2.06	0.55
10:X:194:ASP:HA	10:X:196:GLN:OE1	2.06	0.55
4:D:204:LEU:HD23	4:D:204:LEU:C	2.32	0.55
13:M:171:GLN:NE2	13:M:171:GLN:H	2.05	0.55
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.42	0.55
4:R:6:THR:HG23	5:S:20:GLN:NE2	2.22	0.55
13:a:39:VAL:HA	16:a:359:HOH:O	2.06	0.55
2:B:180:LYS:HE2	2:B:182:ASP:OD1	2.07	0.55
5:E:193:VAL:O	5:E:196:ILE:HG22	2.07	0.55
9:I:17:LYS:HD3	9:I:156:ASN:HD22	1.72	0.55
1:O:28:VAL:HG13	1:O:76:SER:O	2.07	0.55
1:O:57:MET:HE3	1:O:60:THR:HG21	1.89	0.55
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.07	0.55
2:B:239:VAL:HG12	2:B:240:LYS:HD3	1.87	0.54
12:L:159:GLN:HG2	8:V:209:THR:HG21	1.89	0.54
9:W:148:MET:HE2	9:W:172:ASN:HB2	1.89	0.54
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.89	0.54
3:Q:160:GLN:HA	3:Q:160:GLN:NE2	2.17	0.54
6:T:32:THR:HG23	6:T:47:GLU:OE2	2.07	0.54
9:W:123:PHE:N	9:W:123:PHE:CD2	2.75	0.54
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.90	0.54
12:L:121:ALA:HB2	12:L:133:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:93:HIS:CE1	2:P:113:ARG:HD3	2.42	0.54
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.41	0.54
7:G:155:VAL:HG22	7:G:156:GLY:N	2.23	0.54
10:J:194:ASP:HA	10:J:196:GLN:OE1	2.07	0.54
4:R:32:ILE:CD1	4:R:192:VAL:HG23	2.36	0.54
4:R:67:GLY:HA3	4:R:220:PHE:CD2	2.42	0.54
11:Y:4:LEU:CD1	11:Y:161:ILE:HG13	2.38	0.54
12:Z:3:ASN:HD22	12:Z:4:PRO:CD	2.20	0.54
7:G:3:TYR:C	7:G:5:ARG:H	2.15	0.54
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.89	0.54
6:F:172:LEU:O	6:F:176:VAL:HG23	2.07	0.54
16:F:305:HOH:O	7:G:82:ARG:HD2	2.08	0.54
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.73	0.54
1:A:46:ALA:HB2	1:A:211:LEU:HG	1.90	0.54
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.42	0.54
5:S:220:PRO:O	5:S:221:PHE:C	2.51	0.54
8:H:165:ASN:OD1	13:a:153:PRO:HA	2.07	0.54
9:I:124:ASP:HB2	16:I:351:HOH:O	2.08	0.54
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.43	0.54
7:U:119:TYR:CE1	7:U:125:MET:HE2	2.43	0.54
7:U:165:LYS:O	7:U:169:ILE:HG12	2.08	0.54
7:U:201:MET:HA	7:U:201:MET:HE3	1.90	0.54
13:a:197:LEU:HD23	13:a:198:ALA:N	2.23	0.54
14:b:146:MET:HE2	14:b:150:GLU:HB3	1.90	0.54
5:S:207:VAL:HG22	5:S:226:GLY:HA2	1.90	0.54
6:T:8:ASN:CG	6:T:8:ASN:O	2.51	0.54
11:Y:111:THR:HA	16:Y:318:HOH:O	2.08	0.54
13:M:119:VAL:HG23	13:M:200:ILE:CG2	2.34	0.54
8:V:41:ILE:HG13	8:V:76:VAL:HG22	1.89	0.54
13:a:48:ASN:H	13:a:48:ASN:ND2	2.04	0.54
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.90	0.54
1:A:3:ASP:OD2	1:A:5:TYR:HB2	2.08	0.53
3:C:35:LYS:HG2	3:C:158:SER:O	2.08	0.53
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.43	0.53
1:O:46:ALA:HB2	1:O:211:LEU:HG	1.90	0.53
5:S:181:ILE:HG21	5:S:187:GLU:HB2	1.89	0.53
9:W:14:MET:CE	9:W:166:ILE:HG12	2.29	0.53
1:A:59:GLU:H	1:A:59:GLU:CD	2.16	0.53
3:C:222:LEU:HD12	3:C:222:LEU:N	2.24	0.53
5:E:51:ASN:ND2	5:E:53:ASP:O	2.40	0.53
5:E:95:SER:O	5:E:99:ASN:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:PHE:CE1	1:O:209:ILE:HD11	2.42	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.53
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.88	0.53
11:K:4:LEU:CD1	11:K:161:ILE:HG13	2.38	0.53
13:a:161:ARG:HH11	13:a:161:ARG:CG	2.20	0.53
1:A:57:MET:HE3	1:A:60:THR:HG21	1.89	0.53
8:H:41:ILE:HG13	8:H:76:VAL:HG22	1.90	0.53
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.44	0.53
11:Y:111:THR:HG23	16:Y:318:HOH:O	2.09	0.53
13:a:120:GLN:HG3	16:a:348:HOH:O	2.08	0.53
2:B:62:THR:HG22	2:B:65:LEU:O	2.09	0.53
6:F:8:ASN:O	6:F:8:ASN:CG	2.51	0.53
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.39	0.53
1:O:160:LYS:HD3	1:O:179:TRP:CH2	2.44	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.53
9:W:154:GLU:CG	9:W:157:LEU:HD21	2.38	0.53
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.91	0.53
2:P:162:ILE:HG13	2:P:163:SER:N	2.22	0.53
4:R:184:THR:OG1	4:R:187:GLU:HG3	2.07	0.53
7:U:83:ASN:C	7:U:83:ASN:ND2	2.65	0.53
12:Z:3:ASN:ND2	12:Z:5:TYR:H	2.05	0.53
12:Z:121:ALA:HB2	12:Z:133:ARG:NH2	2.22	0.53
1:A:29:LYS:HA	1:A:29:LYS:CE	2.37	0.53
5:E:220:PRO:O	5:E:221:PHE:C	2.52	0.53
6:F:50:ILE:HG13	6:F:208:PHE:HA	1.90	0.53
11:K:78:ALA:O	11:K:82:ILE:HG12	2.08	0.53
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.90	0.53
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.90	0.53
13:a:119:VAL:CG2	13:a:200:ILE:HG22	2.35	0.53
14:b:6:VAL:HG23	14:b:155:ILE:HD11	1.91	0.53
1:A:94:HIS:HD2	8:H:61:SER:OG	1.91	0.53
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.73	0.53
7:G:136:SER:HA	7:G:219:ALA:HB1	1.91	0.53
1:O:29:LYS:HA	1:O:29:LYS:CE	2.38	0.53
2:P:49:ARG:HH22	2:P:61:SER:CB	2.14	0.53
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.44	0.53
3:C:230:TYR:O	3:C:234:ILE:HG13	2.09	0.53
5:S:44:VAL:HG21	5:S:188:LEU:HB3	1.91	0.53
5:S:193:VAL:O	5:S:196:ILE:HG22	2.09	0.53
11:Y:66:HIS:HA	16:Y:335:HOH:O	2.09	0.53
5:E:155:LEU:HD13	5:E:158:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:PHE:CA	5:E:181:ILE:HG12	2.34	0.53
11:K:147:ASP:O	11:K:148:LEU:C	2.50	0.53
5:S:81:ARG:HG3	5:S:81:ARG:NH1	2.23	0.53
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.43	0.53
13:a:227:GLY:HA3	13:a:231:GLN:HB3	1.90	0.53
5:E:64:LYS:HB3	16:E:308:HOH:O	2.09	0.52
8:H:220:ILE:HD11	9:I:194:VAL:HG21	1.92	0.52
11:K:76:VAL:N	11:K:108:GLU:OE2	2.41	0.52
1:O:234:ARG:HG2	1:O:234:ARG:HH11	1.74	0.52
16:D:328:HOH:O	5:E:81:ARG:HD3	2.08	0.52
8:H:29:LYS:HE2	12:Z:194:ARG:CZ	2.40	0.52
8:H:104:ASP:O	8:H:106:THR:N	2.42	0.52
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.44	0.52
13:M:48:ASN:HD22	13:M:48:ASN:N	1.93	0.52
14:N:51:ASP:O	14:N:55:ILE:HG13	2.09	0.52
1:A:160:LYS:HD3	1:A:179:TRP:CH2	2.43	0.52
2:B:24:ALA:O	2:B:28:ILE:HG12	2.09	0.52
7:G:125:MET:HE3	16:G:330:HOH:O	2.09	0.52
8:H:209:THR:HG21	12:Z:159:GLN:HG2	1.91	0.52
10:J:149:ARG:HG2	10:J:149:ARG:HH11	1.73	0.52
2:P:24:ALA:O	2:P:28:ILE:HG12	2.08	0.52
3:Q:174:GLU:OE2	4:R:49:PRO:HD2	2.09	0.52
4:R:51:LEU:HD11	4:R:56:ILE:HD11	1.91	0.52
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.28	0.52
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.91	0.52
7:U:3:TYR:C	7:U:5:ARG:H	2.17	0.52
13:a:171:GLN:NE2	13:a:171:GLN:H	2.08	0.52
4:D:32:ILE:CD1	4:D:192:VAL:HG23	2.37	0.52
7:G:201:MET:HA	7:G:201:MET:HE3	1.92	0.52
4:R:161:ALA:HB3	5:S:55:LEU:CD2	2.38	0.52
10:X:45:SER:OG	10:X:103:LEU:HB2	2.10	0.52
4:D:114:ARG:HH11	4:D:114:ARG:HG2	1.75	0.52
14:N:161:GLN:O	14:N:164:LYS:HB3	2.10	0.52
2:P:228:ILE:HD12	2:P:228:ILE:N	2.25	0.52
5:S:178:PHE:CA	5:S:181:ILE:HG12	2.33	0.52
3:C:174:GLU:OE2	4:D:49:PRO:HD2	2.10	0.52
4:D:67:GLY:HA3	4:D:220:PHE:CE2	2.44	0.52
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.74	0.52
5:S:95:SER:O	5:S:99:ASN:HA	2.08	0.52
6:T:220:THR:O	6:T:221:ASN:HB2	2.09	0.52
7:U:196:PHE:CD1	7:U:196:PHE:C	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLN:CG	3:C:78:ALA:HB1	2.40	0.52
4:D:94:TYR:O	12:L:91:ARG:HG3	2.10	0.52
10:J:1:MET:CG	10:J:2:ASP:H	2.09	0.52
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.91	0.52
4:R:204:LEU:HD23	4:R:205:ASP:N	2.25	0.52
5:S:189:ILE:CG2	5:S:212:ILE:HD13	2.39	0.52
4:D:51:LEU:HD11	4:D:56:ILE:HD11	1.91	0.52
5:E:214:ILE:HG12	5:E:215:VAL:N	2.25	0.52
14:N:9:LYS:HG2	14:N:10:ASP:OD2	2.09	0.52
3:Q:172:PHE:CD2	3:Q:196:SER:HB3	2.45	0.52
12:Z:181:ILE:O	12:Z:185:ARG:HG3	2.10	0.52
13:a:161:ARG:HG3	13:a:161:ARG:NH1	2.21	0.52
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.90	0.52
11:K:15:ALA:O	11:K:161:ILE:HD11	2.10	0.52
6:T:116:VAL:HG21	6:T:147:LEU:HD21	1.91	0.52
3:C:172:PHE:CD2	3:C:196:SER:HB3	2.46	0.51
8:H:73:GLU:OE1	8:H:73:GLU:HA	2.10	0.51
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.51
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.75	0.51
5:S:38:ARG:NH1	5:S:39:SER:O	2.42	0.51
5:S:155:LEU:HD13	5:S:158:THR:HB	1.92	0.51
1:A:29:LYS:HE2	1:A:29:LYS:CA	2.40	0.51
9:I:154:GLU:CG	9:I:157:LEU:HD21	2.40	0.51
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.29	0.51
8:V:18:THR:HB	8:V:30:ASN:HD22	1.76	0.51
13:a:3:GLN:O	13:a:3:GLN:HG3	2.10	0.51
14:b:161:GLN:O	14:b:164:LYS:HB3	2.10	0.51
9:I:176:ARG:NH2	12:Z:147:MET:CE	2.72	0.51
10:J:139:TYR:HE1	16:X:233:HOH:O	1.92	0.51
5:S:1:PHE:O	5:S:3:ASN:N	2.44	0.51
6:T:47:GLU:OE1	6:T:49:LEU:HD21	2.11	0.51
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.10	0.51
5:E:81:ARG:HG3	5:E:81:ARG:NH1	2.24	0.51
13:M:153:PRO:HA	8:V:165:ASN:OD1	2.11	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.91	0.51
2:P:110:LEU:C	2:P:110:LEU:HD23	2.35	0.51
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.93	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.51
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.92	0.51
4:R:67:GLY:HA3	4:R:220:PHE:CE2	2.45	0.51
6:T:191:GLN:HE21	6:T:194:LYS:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:198:ILE:HG23	7:U:214:LEU:HD11	1.92	0.51
2:B:162:ILE:HG13	2:B:163:SER:N	2.25	0.51
1:O:30:GLN:HE21	1:O:30:GLN:CA	2.24	0.51
5:S:214:ILE:HG12	5:S:215:VAL:N	2.25	0.51
6:T:105:ILE:HD12	6:T:105:ILE:N	2.25	0.51
13:a:119:VAL:HG23	13:a:200:ILE:CG2	2.37	0.51
2:B:240:LYS:C	2:B:242:GLY:H	2.19	0.51
4:R:196:LEU:O	4:R:200:MET:HG3	2.10	0.51
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.46	0.51
7:G:83:ASN:C	7:G:83:ASN:ND2	2.69	0.51
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.93	0.51
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.02	0.51
11:Y:32:LYS:N	11:Y:32:LYS:HD2	2.26	0.51
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.91	0.51
13:M:197:LEU:HD23	13:M:198:ALA:N	2.24	0.51
2:P:62:THR:HG22	2:P:65:LEU:O	2.11	0.51
2:P:240:LYS:C	2:P:242:GLY:H	2.18	0.51
10:X:195:PHE:HA	10:X:198:GLN:HB2	1.93	0.51
6:F:47:GLU:OE1	6:F:49:LEU:HD21	2.11	0.51
6:F:116:VAL:HG21	6:F:147:LEU:HD21	1.91	0.51
7:G:165:LYS:O	7:G:169:ILE:HG12	2.11	0.51
11:K:32:LYS:N	11:K:32:LYS:HD2	2.26	0.51
10:X:8:ARG:HG2	10:X:8:ARG:HH11	1.76	0.51
13:a:179:ASN:HB3	16:a:339:HOH:O	2.11	0.51
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.46	0.50
3:C:155:SER:CB	4:D:51:LEU:HD21	2.41	0.50
4:D:210:GLN:HA	16:D:319:HOH:O	2.10	0.50
5:E:90:GLN:HG3	5:E:110:LEU:HD13	1.93	0.50
5:E:189:ILE:CG2	5:E:212:ILE:HD13	2.42	0.50
5:E:227:GLU:N	5:E:227:GLU:CD	2.69	0.50
12:L:147:MET:CE	9:W:176:ARG:NH2	2.74	0.50
6:T:39:ASN:HD22	6:T:39:ASN:N	2.09	0.50
9:W:26:LEU:HD22	9:W:40:GLU:HG2	1.93	0.50
5:E:44:VAL:HG21	5:E:188:LEU:HB3	1.94	0.50
5:E:207:VAL:HG22	5:E:226:GLY:HA2	1.92	0.50
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.44	0.50
3:C:7:SER:O	4:D:128:ARG:HD3	2.12	0.50
4:D:204:LEU:HD23	4:D:205:ASP:N	2.26	0.50
9:I:154:GLU:HG3	9:I:157:LEU:HD21	1.92	0.50
12:L:3:ASN:ND2	12:L:5:TYR:H	2.09	0.50
7:U:155:VAL:HG22	7:U:156:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:LYS:O	14:N:107:LYS:HD3	2.10	0.50
14:N:146:MET:CE	14:N:150:GLU:HB3	2.41	0.50
3:Q:222:LEU:N	3:Q:222:LEU:HD12	2.27	0.50
5:S:36:GLY:O	5:S:157:GLY:HA2	2.10	0.50
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.94	0.50
5:E:174:THR:HG22	5:E:177:THR:HB	1.93	0.50
6:F:49:LEU:HD13	6:F:206:LYS:HD2	1.94	0.50
6:F:105:ILE:HD12	6:F:105:ILE:N	2.26	0.50
4:R:23:ILE:HD13	4:R:133:ALA:HB2	1.94	0.50
5:S:189:ILE:HG23	5:S:212:ILE:HD13	1.94	0.50
7:U:186:ASN:C	7:U:186:ASN:HD22	2.18	0.50
9:W:22:ILE:HG12	9:W:42:ILE:HD12	1.94	0.50
14:b:116:GLY:HA3	16:b:203:HOH:O	2.12	0.50
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.27	0.50
1:A:128:ARG:NH2	7:G:120:THR:HG22	2.15	0.50
5:E:1:PHE:O	5:E:3:ASN:N	2.45	0.50
7:G:198:ILE:HG23	7:G:214:LEU:HD11	1.92	0.50
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.94	0.50
2:B:185:VAL:O	2:B:189:ILE:HG13	2.11	0.50
5:E:38:ARG:NH1	5:E:39:SER:O	2.44	0.50
1:O:94:HIS:HD2	8:V:61:SER:OG	1.94	0.50
2:P:67:LYS:HG3	2:P:226:GLN:OE1	2.11	0.50
6:T:49:LEU:HD13	6:T:206:LYS:HD2	1.92	0.50
7:U:136:SER:HA	7:U:219:ALA:HB1	1.93	0.50
14:b:9:LYS:O	14:b:107:LYS:HD3	2.12	0.50
4:D:23:ILE:HD13	4:D:133:ALA:HB2	1.94	0.50
7:G:186:ASN:HD22	7:G:186:ASN:C	2.19	0.50
13:M:48:ASN:N	13:M:48:ASN:ND2	2.60	0.50
2:P:55:LEU:HD22	2:P:55:LEU:H	1.76	0.50
4:R:114:ARG:HG2	4:R:114:ARG:HH11	1.76	0.50
16:R:316:HOH:O	12:Z:95:HIS:HD2	1.94	0.50
8:V:34:LEU:HB2	16:V:317:HOH:O	2.11	0.50
9:W:50:LEU:HD21	9:W:52:ILE:HD11	1.94	0.50
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.93	0.50
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.47	0.50
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.93	0.50
7:G:196:PHE:CD1	7:G:196:PHE:C	2.88	0.50
8:H:152:ILE:O	8:H:156:SER:HB2	2.12	0.50
9:I:22:ILE:HG12	9:I:42:ILE:HD12	1.93	0.50
10:J:173:PRO:O	10:X:174:MET:HE2	2.11	0.50
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:3:GLN:HG3	13:M:3:GLN:O	2.12	0.50
2:B:149:THR:O	2:B:156:TYR:HA	2.12	0.49
12:L:152:ASN:O	12:L:156:PHE:HA	2.12	0.49
4:R:6:THR:HG22	4:R:7:PHE:N	2.26	0.49
6:T:123:ASN:HD22	6:T:123:ASN:C	2.20	0.49
9:W:179:LEU:HD22	16:W:313:HOH:O	2.12	0.49
14:b:175:MET:HB2	14:b:186:LEU:HB2	1.92	0.49
5:E:227:GLU:CD	5:E:227:GLU:H	2.20	0.49
10:J:195:PHE:HA	10:J:198:GLN:HB2	1.94	0.49
12:L:194:ARG:CZ	8:V:29:LYS:HE2	2.41	0.49
14:N:103:ASP:HB2	16:N:234:HOH:O	2.12	0.49
2:P:120:GLY:C	2:P:122:THR:H	2.20	0.49
5:S:90:GLN:HG3	5:S:110:LEU:HD13	1.94	0.49
5:S:227:GLU:CD	5:S:227:GLU:N	2.69	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.10	0.49
4:D:6:THR:HG22	4:D:7:PHE:N	2.26	0.49
1:O:160:LYS:HD3	1:O:179:TRP:CZ3	2.47	0.49
1:O:205:ASN:HB2	16:O:329:HOH:O	2.12	0.49
5:S:174:THR:HG22	5:S:177:THR:HB	1.92	0.49
6:T:105:ILE:HD13	6:T:138:ASP:HB3	1.93	0.49
8:V:104:ASP:O	8:V:106:THR:N	2.45	0.49
11:Y:15:ALA:O	11:Y:161:ILE:HD11	2.12	0.49
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.93	0.49
1:A:24:ALA:O	1:A:28:VAL:HG23	2.13	0.49
2:B:110:LEU:HD23	2:B:110:LEU:C	2.36	0.49
12:L:100:LYS:HD3	12:L:105:TYR:CE1	2.47	0.49
12:L:181:ILE:O	12:L:185:ARG:HG3	2.12	0.49
13:M:18:ASN:HB3	13:M:201:ASP:OD2	2.12	0.49
3:Q:27:ARG:NH1	3:Q:27:ARG:HB2	2.27	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.95	0.49
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.94	0.49
8:V:73:GLU:OE1	8:V:73:GLU:HA	2.12	0.49
11:Y:145:LYS:O	11:Y:148:LEU:HD13	2.12	0.49
6:F:175:LEU:HD11	6:F:191:GLN:HG3	1.94	0.49
10:J:174:MET:HG2	10:X:174:MET:CE	2.43	0.49
12:L:94:GLN:HG3	12:L:129:GLY:O	2.11	0.49
1:A:160:LYS:HD3	1:A:179:TRP:CZ3	2.47	0.49
7:G:174:GLU:O	7:G:178:LYS:HG3	2.12	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.49
1:O:24:ALA:O	1:O:28:VAL:HG23	2.12	0.49
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:THR:CG2	10:J:54:VAL:H	2.25	0.49
4:R:155:THR:HG23	5:S:78:PRO:HD3	1.94	0.49
6:T:193:ALA:O	6:T:197:TYR:HD1	1.95	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
12:Z:94:GLN:HG3	12:Z:129:GLY:O	2.12	0.49
4:D:121:GLY:HA3	16:E:315:HOH:O	2.13	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.49
5:E:189:ILE:HG23	5:E:212:ILE:HD13	1.95	0.49
11:K:12:ILE:HG23	11:K:112:ILE:HD11	1.94	0.49
5:S:214:ILE:O	5:S:221:PHE:HA	2.13	0.49
6:T:191:GLN:NE2	6:T:194:LYS:CE	2.76	0.49
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.93	0.49
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.95	0.49
11:K:12:ILE:CG2	11:K:112:ILE:HD11	2.43	0.49
3:Q:190:VAL:HG13	3:Q:210:ILE:HG21	1.94	0.49
5:S:174:THR:HG22	5:S:174:THR:O	2.13	0.49
5:E:214:ILE:O	5:E:221:PHE:HA	2.13	0.49
6:F:193:ALA:O	6:F:197:TYR:HD1	1.96	0.49
10:J:198:GLN:OXT	10:J:198:GLN:HG2	2.12	0.49
13:M:48:ASN:H	13:M:48:ASN:ND2	2.02	0.49
10:J:45:SER:OG	10:J:103:LEU:HB2	2.13	0.48
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.12	0.48
14:N:67:THR:HA	14:N:71:GLY:O	2.13	0.48
2:P:148:TYR:CZ	3:Q:57:ILE:HG13	2.47	0.48
16:T:303:HOH:O	7:U:82:ARG:HD2	2.12	0.48
9:W:17:LYS:CD	9:W:156:ASN:HD22	2.26	0.48
6:F:45:ALA:HA	6:F:211:GLU:O	2.12	0.48
6:F:191:GLN:HE21	6:F:194:LYS:HE3	1.78	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.48	0.48
1:O:139:HIS:HA	1:O:144:GLY:O	2.13	0.48
1:O:246:ARG:HG3	1:O:246:ARG:NH1	2.28	0.48
9:W:28:LEU:HA	16:W:316:HOH:O	2.12	0.48
10:X:198:GLN:OXT	10:X:198:GLN:HG2	2.13	0.48
2:B:228:ILE:N	2:B:228:ILE:HD12	2.28	0.48
5:E:14:PRO:HA	6:F:22:TYR:CD2	2.48	0.48
5:E:174:THR:HG22	5:E:174:THR:O	2.12	0.48
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.43	0.48
9:I:26:LEU:HD22	9:I:40:GLU:HG2	1.94	0.48
2:P:6:ASP:OD1	3:Q:4:ARG:HG3	2.12	0.48
4:R:82:GLU:OE1	11:Y:69:ARG:HD2	2.13	0.48
5:S:227:GLU:CD	5:S:227:GLU:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:53:THR:CG2	10:X:54:VAL:H	2.26	0.48
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	1.95	0.48
12:Z:100:LYS:HD3	12:Z:105:TYR:CE1	2.47	0.48
2:B:55:LEU:HD22	2:B:55:LEU:H	1.75	0.48
2:B:67:LYS:HG3	2:B:226:GLN:OE1	2.14	0.48
2:B:120:GLY:C	2:B:122:THR:H	2.21	0.48
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.94	0.48
10:J:53:THR:HG23	10:J:54:VAL:HG23	1.95	0.48
1:O:54:PRO:HG2	7:U:174:GLU:HG2	1.95	0.48
2:P:149:THR:O	2:P:156:TYR:HA	2.13	0.48
2:P:162:ILE:HG13	2:P:163:SER:H	1.79	0.48
2:P:185:VAL:O	2:P:189:ILE:HG13	2.13	0.48
3:Q:29:THR:HB	3:Q:45:GLU:HG3	1.96	0.48
3:Q:182:PRO:O	3:Q:184:ALA:N	2.46	0.48
3:Q:239:GLN:C	3:Q:241:GLN:H	2.22	0.48
4:R:4:VAL:CG2	4:R:116:GLY:HA2	2.44	0.48
14:b:41:ILE:HD12	14:b:75:THR:HA	1.95	0.48
5:E:36:GLY:O	5:E:157:GLY:HA2	2.12	0.48
6:F:20:VAL:O	6:F:23:ALA:HB3	2.13	0.48
8:H:128:GLY:O	8:H:131:SER:HB2	2.13	0.48
2:P:184:LYS:HD3	2:P:185:VAL:H	1.75	0.48
4:R:93:LEU:CD1	11:Y:57:THR:HG22	2.43	0.48
9:W:106:PRO:HB2	9:W:123:PHE:CD2	2.48	0.48
13:a:18:ASN:HB3	13:a:201:ASP:OD2	2.13	0.48
4:D:4:VAL:CG2	4:D:116:GLY:HA2	2.43	0.48
9:I:10:ILE:HD11	9:I:174:ALA:HB2	1.96	0.48
14:N:136:GLY:HA2	14:b:161:GLN:NE2	2.11	0.48
6:T:45:ALA:HA	6:T:211:GLU:O	2.13	0.48
7:U:235:ARG:NE	7:U:235:ARG:HA	2.29	0.48
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.94	0.48
14:b:67:THR:HA	14:b:71:GLY:O	2.14	0.48
7:G:101:TYR:OH	8:H:66:HIS:HE1	1.97	0.48
8:H:18:THR:HB	8:H:30:ASN:HD22	1.79	0.48
11:K:145:LYS:O	11:K:148:LEU:HD13	2.13	0.48
3:Q:49:THR:HG22	3:Q:50:LEU:HD22	1.95	0.48
6:T:175:LEU:HD11	6:T:191:GLN:HG3	1.95	0.48
8:V:84:LYS:HG3	8:V:85:GLN:N	2.28	0.48
10:X:49:GLU:HB2	10:X:99:GLN:HB2	1.96	0.48
11:Y:12:ILE:CG2	11:Y:112:ILE:HD11	2.43	0.48
14:b:9:LYS:HG2	14:b:10:ASP:OD2	2.13	0.48
3:C:239:GLN:C	3:C:241:GLN:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:GLY:HA3	7:G:224:PHE:CE2	2.49	0.48
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.95	0.48
10:J:174:MET:CE	10:X:174:MET:HG2	2.43	0.48
8:V:220:ILE:HD11	9:W:194:VAL:HG21	1.96	0.48
10:X:13:VAL:HG23	10:X:114:PRO:HB2	1.95	0.48
2:B:184:LYS:HD3	2:B:185:VAL:H	1.77	0.48
3:C:29:THR:HB	3:C:45:GLU:HG3	1.95	0.48
9:I:50:LEU:HD21	9:I:52:ILE:HD11	1.95	0.48
10:J:172:MET:CE	10:J:174:MET:HB2	2.44	0.48
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.95	0.48
7:U:166:GLN:NE2	7:U:167:GLN:N	2.62	0.48
1:A:139:HIS:HA	1:A:144:GLY:O	2.13	0.48
14:N:41:ILE:HD12	14:N:75:THR:HA	1.96	0.48
14:b:146:MET:CE	14:b:150:GLU:HB3	2.44	0.48
1:A:206:GLY:HA2	1:A:243:ILE:HG21	1.96	0.47
6:F:39:ASN:HD22	6:F:39:ASN:N	2.10	0.47
8:H:175:VAL:HG12	8:H:176:CYS:N	2.29	0.47
4:R:176:LEU:HD22	5:S:55:LEU:HD11	1.95	0.47
10:X:118:GLN:NE2	10:X:132:ALA:H	2.11	0.47
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.39	0.47
3:C:182:PRO:O	3:C:184:ALA:N	2.48	0.47
14:N:107:LYS:HG2	14:N:108:GLY:H	1.79	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.47
6:T:20:VAL:O	6:T:23:ALA:HB3	2.14	0.47
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.96	0.47
13:a:129:TYR:CE1	13:a:144:THR:HG22	2.48	0.47
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.15	0.47
3:C:160:GLN:HA	3:C:160:GLN:NE2	2.18	0.47
5:E:86:TYR:CD1	5:E:114:LYS:HD2	2.50	0.47
6:F:191:GLN:O	6:F:195:ILE:HG13	2.14	0.47
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.96	0.47
9:I:108:VAL:O	9:I:120:ILE:HA	2.14	0.47
10:J:8:ARG:HG2	10:J:8:ARG:HH11	1.79	0.47
1:O:206:GLY:HA2	1:O:243:ILE:HG21	1.96	0.47
3:Q:32:VAL:HG22	3:Q:33:GLY:N	2.29	0.47
4:R:241:ALA:O	4:R:242:GLU:CB	2.62	0.47
6:T:168:ALA:O	6:T:172:LEU:HD23	2.15	0.47
7:U:19:VAL:O	7:U:23:PHE:HD2	1.97	0.47
7:U:39:LYS:NZ	7:U:186:ASN:ND2	2.62	0.47
7:U:148:THR:HG22	7:U:154:TYR:HB2	1.96	0.47
9:W:108:VAL:O	9:W:120:ILE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:MET:HE2	2:B:145:TYR:O	2.14	0.47
7:G:119:TYR:CE1	7:G:125:MET:HE2	2.49	0.47
13:M:40:GLU:OE1	13:M:42:LEU:HB2	2.14	0.47
4:R:113:LEU:HD13	5:S:125:ARG:NH2	2.29	0.47
6:T:183:LEU:HD11	6:T:187:GLU:HB3	1.97	0.47
9:W:55:LEU:HG	9:W:57:THR:HG22	1.96	0.47
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.97	0.47
10:J:173:PRO:HB2	10:X:174:MET:HE1	1.97	0.47
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.50	0.47
13:M:172:VAL:HG21	16:M:359:HOH:O	2.14	0.47
2:P:99:LYS:NZ	10:X:86:GLN:NE2	2.61	0.47
3:Q:170:ARG:O	3:Q:174:GLU:HG3	2.15	0.47
4:R:121:GLY:O	4:R:122:GLU:HB2	2.13	0.47
5:S:200:LEU:HD11	5:S:205:LEU:CD2	2.40	0.47
10:X:61:GLN:HB3	16:X:236:HOH:O	2.13	0.47
3:C:117:ARG:NH2	16:C:327:HOH:O	2.45	0.47
4:D:121:GLY:O	4:D:122:GLU:HB2	2.14	0.47
6:F:183:LEU:HD11	6:F:187:GLU:HB3	1.97	0.47
10:J:172:MET:HA	10:J:173:PRO:HD3	1.79	0.47
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.97	0.47
14:N:102:TYR:OH	14:N:180:ALA:HB2	2.14	0.47
6:T:191:GLN:O	6:T:195:ILE:HG13	2.15	0.47
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.80	0.47
12:Z:109:THR:CG2	16:Z:311:HOH:O	2.63	0.47
14:b:13:ILE:HG12	14:b:177:VAL:HG13	1.95	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.14	0.47
2:B:142:ARG:NH1	10:J:73:TYR:HB2	2.29	0.47
4:D:196:LEU:O	4:D:200:MET:HG3	2.15	0.47
16:F:305:HOH:O	7:G:79:PRO:HA	2.14	0.47
9:I:55:LEU:HG	9:I:57:THR:HG22	1.95	0.47
11:K:208:ASN:HD21	10:X:150:PRO:CG	2.28	0.47
2:P:229:PHE:N	2:P:229:PHE:CD2	2.83	0.47
3:Q:39:CYS:HA	3:Q:136:PHE:HZ	1.80	0.47
3:Q:51:LYS:NZ	3:Q:52:LEU:HA	2.30	0.47
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.43	0.47
10:X:172:MET:HA	10:X:173:PRO:HD3	1.79	0.47
1:A:231:LYS:HE3	16:A:347:HOH:O	2.13	0.47
3:C:49:THR:HG22	3:C:50:LEU:HD22	1.97	0.47
3:C:190:VAL:HG13	3:C:210:ILE:HG21	1.96	0.47
5:E:69:MET:CE	5:E:104:VAL:HA	2.44	0.47
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:166:ILE:HG22	9:I:167:SER:N	2.30	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
3:Q:49:THR:HG22	3:Q:50:LEU:CD2	2.44	0.47
3:Q:160:GLN:CA	3:Q:160:GLN:NE2	2.77	0.47
6:T:191:GLN:NE2	6:T:194:LYS:HE2	2.29	0.47
7:U:72:MET:HE3	7:U:74:VAL:CG2	2.45	0.47
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.40	0.47
2:B:243:ILE:O	2:B:243:ILE:HG22	2.15	0.47
3:C:27:ARG:NH1	3:C:27:ARG:HB2	2.29	0.47
6:F:8:ASN:OD1	6:F:127:PRO:HG3	2.15	0.47
6:F:105:ILE:HD13	6:F:138:ASP:HB3	1.97	0.47
10:J:174:MET:HE2	10:X:173:PRO:O	2.15	0.47
11:K:208:ASN:HD21	10:X:150:PRO:HG2	1.79	0.47
12:L:2:PHE:CB	13:M:1:THR:HG23	2.45	0.47
6:T:210:LEU:HD21	6:T:212:ILE:HD11	1.97	0.47
9:W:137:VAL:CG1	9:W:145:LEU:HB3	2.45	0.47
3:C:32:VAL:HG22	3:C:33:GLY:N	2.28	0.47
4:D:241:ALA:O	4:D:242:GLU:CB	2.63	0.47
5:E:69:MET:HE2	5:E:104:VAL:HA	1.97	0.47
6:F:132:THR:O	6:F:146:MET:HA	2.15	0.47
7:G:191:GLU:O	7:G:195:GLU:HG3	2.15	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.47
13:a:169:THR:HG23	16:a:322:HOH:O	2.15	0.47
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.28	0.46
6:F:191:GLN:NE2	6:F:194:LYS:CE	2.78	0.46
8:H:84:LYS:HG3	8:H:85:GLN:N	2.30	0.46
13:a:48:ASN:N	13:a:48:ASN:ND2	2.62	0.46
3:C:51:LYS:NZ	3:C:52:LEU:HA	2.29	0.46
4:D:140:ASP:HA	16:D:338:HOH:O	2.16	0.46
5:E:200:LEU:HD11	5:E:205:LEU:CD2	2.42	0.46
16:E:305:HOH:O	6:F:8:ASN:HB2	2.16	0.46
2:P:49:ARG:NH2	2:P:58:GLN:HE21	2.12	0.46
5:S:181:ILE:HG22	5:S:181:ILE:O	2.15	0.46
1:A:28:VAL:HG13	1:A:76:SER:O	2.15	0.46
2:B:229:PHE:CD2	2:B:229:PHE:N	2.83	0.46
5:E:21:VAL:O	5:E:25:LEU:HD13	2.15	0.46
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.46	0.46
9:W:50:LEU:CG	9:W:52:ILE:HD11	2.46	0.46
10:X:172:MET:CE	10:X:174:MET:HB2	2.45	0.46
1:A:69:PRO:HD3	16:H:352:HOH:O	2.14	0.46
1:A:238:LEU:HA	1:A:242:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:CZ	2:B:58:GLN:HE21	2.28	0.46
5:E:23:TYR:O	5:E:26:GLU:HB3	2.16	0.46
6:F:123:ASN:HD22	6:F:123:ASN:C	2.22	0.46
7:G:135:VAL:HA	7:G:144:SER:O	2.15	0.46
12:L:89:ALA:O	12:L:93:ILE:HG12	2.16	0.46
12:L:125:PHE:N	12:L:125:PHE:CD1	2.82	0.46
1:O:52:SER:O	1:O:53:SER:HB2	2.15	0.46
7:U:135:VAL:HA	7:U:144:SER:O	2.15	0.46
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.96	0.46
8:V:175:VAL:HG12	8:V:176:CYS:N	2.30	0.46
11:Y:176:ASN:HD21	11:Y:190:ASN:HB2	1.80	0.46
2:B:49:ARG:NH2	2:B:58:GLN:HE21	2.13	0.46
2:B:139:TYR:CG	2:B:224:VAL:HG21	2.51	0.46
6:F:105:ILE:N	6:F:106:PRO:CD	2.79	0.46
8:H:104:ASP:C	8:H:106:THR:H	2.23	0.46
9:I:106:PRO:HB2	9:I:123:PHE:CD2	2.50	0.46
10:J:49:GLU:HB2	10:J:99:GLN:HB2	1.97	0.46
12:L:108:HIS:HE1	12:L:124:SER:HB2	1.81	0.46
1:O:238:LEU:HA	1:O:242:GLU:OE1	2.15	0.46
14:b:84:GLU:O	14:b:88:GLU:HB2	2.16	0.46
7:G:235:ARG:NE	7:G:235:ARG:HA	2.30	0.46
10:J:75:LEU:HD22	10:J:79:ALA:HB1	1.97	0.46
11:K:140:LEU:HD13	11:K:160:SER:OG	2.16	0.46
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.97	0.46
5:S:23:TYR:O	5:S:26:GLU:HB3	2.14	0.46
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.51	0.46
7:U:71:GLY:HA3	7:U:224:PHE:CE2	2.50	0.46
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.98	0.46
7:U:137:VAL:HG21	7:U:220:THR:HA	1.97	0.46
8:V:152:ILE:O	8:V:156:SER:HB2	2.14	0.46
11:Y:12:ILE:HD13	11:Y:112:ILE:HD13	1.97	0.46
12:Z:2:PHE:CB	13:a:1:THR:HG23	2.44	0.46
13:a:40:GLU:OE1	13:a:42:LEU:HB2	2.16	0.46
1:A:52:SER:O	1:A:53:SER:HB2	2.14	0.46
2:B:17:ARG:HG2	2:B:17:ARG:NH1	2.31	0.46
3:C:225:GLU:OE1	3:C:225:GLU:N	2.48	0.46
6:F:168:ALA:O	6:F:172:LEU:HD23	2.15	0.46
6:F:191:GLN:NE2	6:F:194:LYS:HE2	2.31	0.46
13:M:165:ILE:N	13:M:166:PRO:HD2	2.31	0.46
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.46	0.46
7:U:192:LYS:HD3	7:U:195:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:130:TYR:CD2	10:X:144:LEU:HD13	2.51	0.46
3:C:100:ASP:OD2	3:C:101:PRO:HD2	2.16	0.46
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.45	0.46
5:E:35:VAL:HG12	5:E:36:GLY:N	2.31	0.46
9:I:124:ASP:HB3	15:c:2:THR:HG23	1.98	0.46
10:J:129:PRO:HB2	10:J:130:TYR:CD1	2.50	0.46
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.98	0.46
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.97	0.46
12:Z:10:GLY:HA3	12:Z:42:LYS:NZ	2.30	0.46
4:D:214:ILE:O	4:D:214:ILE:HG23	2.15	0.46
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.97	0.46
5:E:131:LEU:HD12	5:E:146:PHE:CD2	2.51	0.46
11:K:185:TRP:C	11:K:186:ILE:HD13	2.41	0.46
2:P:49:ARG:CZ	2:P:58:GLN:HE21	2.29	0.46
14:b:102:TYR:OH	14:b:180:ALA:HB2	2.16	0.46
1:A:205:ASN:HA	1:A:247:LEU:CD1	2.45	0.46
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.16	0.46
10:J:194:ASP:O	10:J:198:GLN:HB2	2.16	0.46
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.80	0.46
3:Q:100:ASP:OD2	3:Q:101:PRO:HD2	2.16	0.46
6:T:103:ILE:HG12	6:T:108:PHE:HB2	1.98	0.46
12:Z:3:ASN:HD22	12:Z:3:ASN:C	2.22	0.46
12:Z:3:ASN:ND2	12:Z:3:ASN:C	2.72	0.46
6:T:41:GLY:HA3	6:T:215:CYS:O	2.15	0.45
6:T:99:TYR:O	6:T:100:LYS:HB3	2.15	0.45
6:T:201:GLU:O	6:T:204:LYS:HD2	2.16	0.45
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.46	0.45
11:Y:185:TRP:C	11:Y:186:ILE:HD13	2.41	0.45
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.29	0.45
1:A:10:THR:O	2:B:128:ARG:HD3	2.16	0.45
2:B:234:ILE:HD11	16:B:316:HOH:O	2.16	0.45
3:C:227:ILE:O	3:C:231:VAL:HG23	2.16	0.45
4:D:44:LYS:HB2	4:D:208:ASN:C	2.41	0.45
7:G:192:LYS:HD3	7:G:195:GLU:OE2	2.15	0.45
12:L:103:PHE:N	12:L:104:PRO:CD	2.80	0.45
14:b:51:ASP:O	14:b:55:ILE:HG13	2.16	0.45
2:B:183:MET:HE1	2:B:188:ALA:HA	1.98	0.45
3:C:39:CYS:HA	3:C:136:PHE:HZ	1.81	0.45
7:G:132:LEU:O	7:G:147:LYS:HA	2.15	0.45
9:I:20:VAL:CG1	9:I:118:PRO:HB3	2.47	0.45
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:148:LYS:O	8:V:152:ILE:HG13	2.16	0.45
5:E:72:SER:OG	5:E:132:LEU:HB2	2.16	0.45
4:R:6:THR:CG2	4:R:7:PHE:N	2.80	0.45
5:S:37:LEU:N	5:S:37:LEU:HD23	2.31	0.45
6:T:201:GLU:C	6:T:203:ASN:H	2.24	0.45
11:K:4:LEU:HD22	11:K:4:LEU:C	2.41	0.45
1:O:97:TYR:OH	9:W:77:GLU:OE2	2.33	0.45
2:P:135:ILE:HD11	2:P:164:VAL:HG22	1.99	0.45
4:R:44:LYS:HB2	4:R:208:ASN:C	2.42	0.45
6:T:237:ASP:O	6:T:238:PHE:C	2.60	0.45
13:a:206:LEU:HD23	13:a:206:LEU:C	2.41	0.45
7:G:137:VAL:HG21	7:G:220:THR:HA	1.97	0.45
10:J:118:GLN:NE2	10:J:132:ALA:H	2.15	0.45
13:M:206:LEU:HD23	13:M:206:LEU:C	2.42	0.45
5:S:167:ALA:HB2	5:S:195:ALA:O	2.15	0.45
16:S:309:HOH:O	6:T:8:ASN:HB2	2.16	0.45
7:U:132:LEU:O	7:U:147:LYS:HA	2.15	0.45
11:Y:140:LEU:HD13	11:Y:160:SER:OG	2.16	0.45
1:A:64:VAL:HG11	1:A:212:ALA:HB3	1.99	0.45
6:F:36:ILE:HD12	6:F:192:ALA:HB2	1.98	0.45
7:G:231:ASN:N	7:G:231:ASN:HD22	2.14	0.45
9:I:80:ALA:HB1	16:I:326:HOH:O	2.17	0.45
11:K:208:ASN:ND2	10:X:150:PRO:CG	2.80	0.45
13:M:161:ARG:HH11	13:M:161:ARG:CG	2.20	0.45
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.16	0.45
4:R:73:LEU:HB3	16:R:308:HOH:O	2.16	0.45
4:R:214:ILE:O	4:R:214:ILE:HG23	2.15	0.45
5:S:9:THR:HG21	5:S:126:PRO:HG3	1.99	0.45
6:T:39:ASN:N	6:T:39:ASN:ND2	2.64	0.45
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.81	0.45
5:E:37:LEU:N	5:E:37:LEU:HD23	2.32	0.45
5:E:129:VAL:O	5:E:148:PRO:HG3	2.16	0.45
9:I:50:LEU:CG	9:I:52:ILE:HD11	2.47	0.45
11:K:12:ILE:HD13	11:K:112:ILE:HD13	1.98	0.45
12:L:10:GLY:HA3	12:L:42:LYS:NZ	2.31	0.45
12:L:30:ILE:C	12:L:30:ILE:CD1	2.90	0.45
1:O:29:LYS:HE2	1:O:29:LYS:CA	2.41	0.45
1:O:248:GLU:C	1:O:250:LEU:N	2.75	0.45
6:T:172:LEU:HB3	7:U:54:LEU:HD21	1.98	0.45
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.99	0.45
12:Z:51:VAL:HG23	12:Z:112:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:SER:HB2	16:C:311:HOH:O	2.17	0.45
5:E:167:ALA:HB2	5:E:195:ALA:O	2.17	0.45
7:G:39:LYS:NZ	7:G:186:ASN:ND2	2.65	0.45
2:P:240:LYS:C	2:P:242:GLY:N	2.75	0.45
2:P:243:ILE:O	2:P:243:ILE:HG22	2.17	0.45
3:Q:165:ASN:CB	3:Q:200:VAL:HG11	2.45	0.45
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.99	0.45
8:V:104:ASP:C	8:V:106:THR:H	2.24	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.45
9:W:68:TYR:CD1	9:W:68:TYR:C	2.95	0.45
10:X:75:LEU:HD22	10:X:79:ALA:HB1	1.97	0.45
2:B:162:ILE:HG13	2:B:163:SER:H	1.81	0.45
3:C:49:THR:HG22	3:C:50:LEU:CD2	2.46	0.45
7:G:232:ILE:O	7:G:235:ARG:N	2.50	0.45
10:J:13:VAL:HG23	10:J:114:PRO:HB2	1.98	0.45
11:K:86:LEU:HD13	11:K:86:LEU:C	2.42	0.45
1:O:59:GLU:C	1:O:61:LEU:H	2.24	0.45
1:O:203:GLU:OE2	1:O:203:GLU:HA	2.17	0.45
3:Q:51:LYS:HZ2	3:Q:52:LEU:HA	1.81	0.45
4:R:113:LEU:HD13	5:S:125:ARG:HH21	1.82	0.45
5:S:69:MET:CE	5:S:104:VAL:HA	2.47	0.45
8:V:38:SER:OG	8:V:41:ILE:HD13	2.17	0.45
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.16	0.45
10:X:139:TYR:CZ	10:X:172:MET:HG3	2.51	0.45
11:Y:174:SER:HA	11:Y:193:VAL:HG23	1.99	0.45
12:Z:109:THR:HG23	16:Z:311:HOH:O	2.16	0.45
13:a:17:ASP:HB3	13:a:166:PRO:HA	1.99	0.45
13:a:162:GLU:O	13:a:165:ILE:HG13	2.17	0.45
13:a:165:ILE:N	13:a:166:PRO:HD2	2.32	0.45
14:b:179:THR:HB	16:b:244:HOH:O	2.16	0.45
3:C:1:GLY:N	16:C:330:HOH:O	2.50	0.44
4:D:31:GLY:O	4:D:161:ALA:HA	2.18	0.44
9:I:137:VAL:CG1	9:I:145:LEU:HB3	2.47	0.44
12:L:41:PRO:HA	16:L:345:HOH:O	2.17	0.44
3:Q:27:ARG:HB2	3:Q:27:ARG:CZ	2.46	0.44
4:R:176:LEU:HD22	5:S:55:LEU:CD1	2.47	0.44
5:S:72:SER:OG	5:S:132:LEU:HB2	2.17	0.44
6:T:8:ASN:OD1	6:T:127:PRO:HG3	2.17	0.44
9:W:50:LEU:HG	9:W:52:ILE:CD1	2.47	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.99	0.44
4:D:9:PRO:HD2	16:D:331:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:TYR:O	6:F:100:LYS:HB3	2.17	0.44
14:N:156:LYS:HG2	14:N:196:LEU:HD11	1.99	0.44
3:Q:227:ILE:O	3:Q:231:VAL:HG23	2.17	0.44
4:R:9:PRO:HA	5:S:23:TYR:CD2	2.51	0.44
1:A:59:GLU:C	1:A:61:LEU:H	2.25	0.44
3:C:165:ASN:CB	3:C:200:VAL:HG11	2.46	0.44
5:E:101:LYS:HA	16:E:302:HOH:O	2.17	0.44
6:F:103:ILE:HG12	6:F:108:PHE:HB2	1.99	0.44
10:J:174:MET:HE3	10:X:174:MET:HG2	1.98	0.44
11:K:174:SER:HA	11:K:193:VAL:HG23	1.99	0.44
14:N:146:MET:HE2	14:N:150:GLU:C	2.42	0.44
16:N:227:HOH:O	13:a:233:ILE:HD11	2.16	0.44
2:P:183:MET:HE1	2:P:188:ALA:HA	1.99	0.44
3:Q:107:LEU:HD13	3:Q:107:LEU:O	2.17	0.44
5:S:69:MET:HE2	5:S:104:VAL:HA	1.97	0.44
12:Z:42:LYS:HD2	12:Z:55:ASN:ND2	2.32	0.44
13:a:11:VAL:O	13:a:143:ALA:HA	2.18	0.44
2:B:60:THR:HG22	2:B:60:THR:O	2.18	0.44
6:F:39:ASN:N	6:F:39:ASN:ND2	2.66	0.44
6:F:201:GLU:C	6:F:203:ASN:H	2.24	0.44
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.99	0.44
8:H:148:LYS:O	8:H:152:ILE:HG13	2.17	0.44
10:J:174:MET:HG2	10:X:174:MET:HE3	1.99	0.44
10:J:190:ARG:HA	16:J:247:HOH:O	2.18	0.44
13:M:25:ASP:HA	13:M:195:PHE:HA	2.00	0.44
2:P:50:LYS:HG2	2:P:51:VAL:HG23	1.99	0.44
5:S:21:VAL:O	5:S:25:LEU:HD13	2.17	0.44
5:S:73:LEU:C	5:S:73:LEU:HD12	2.43	0.44
6:T:138:ASP:C	6:T:138:ASP:OD2	2.61	0.44
7:U:237:VAL:O	7:U:240:ALA:HB3	2.18	0.44
12:Z:125:PHE:N	12:Z:125:PHE:CD1	2.85	0.44
14:b:163:ILE:HG23	14:b:170:GLY:HA2	2.00	0.44
2:B:24:ALA:O	2:B:27:SER:HB3	2.18	0.44
2:B:50:LYS:HG2	2:B:51:VAL:HG23	1.98	0.44
4:D:6:THR:CG2	4:D:7:PHE:N	2.80	0.44
10:J:139:TYR:HD1	16:Y:317:HOH:O	2.00	0.44
13:M:17:ASP:HB3	13:M:166:PRO:HA	1.98	0.44
2:P:69:ASN:CG	2:P:70:ASP:H	2.23	0.44
5:S:102:LEU:HA	16:S:321:HOH:O	2.18	0.44
7:U:191:GLU:O	7:U:195:GLU:HG3	2.17	0.44
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.18	0.44
12:Z:38:ARG:NH1	12:Z:221:ARG:HB3	2.33	0.44
3:C:95:ARG:HH11	3:C:101:PRO:HB3	1.82	0.44
5:E:181:ILE:HG22	5:E:181:ILE:O	2.17	0.44
9:I:17:LYS:CD	9:I:156:ASN:HD22	2.29	0.44
11:K:15:ALA:C	11:K:161:ILE:HD11	2.42	0.44
13:M:161:ARG:HG3	13:M:161:ARG:NH1	2.20	0.44
3:Q:40:VAL:HG22	3:Q:143:PRO:HB2	2.00	0.44
5:S:129:VAL:O	5:S:148:PRO:HG3	2.18	0.44
9:W:166:ILE:HG22	9:W:167:SER:N	2.31	0.44
13:a:150:MET:C	13:a:153:PRO:HD2	2.42	0.44
4:D:200:MET:HB3	4:D:200:MET:HE2	1.81	0.44
5:E:99:ASN:HB2	13:M:94:GLU:CG	2.46	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.21	0.44
11:K:46:ALA:HB3	11:K:98:GLY:O	2.18	0.44
12:L:3:ASN:HD22	12:L:3:ASN:C	2.26	0.44
13:M:88:GLU:HB2	13:M:91:TYR:CD2	2.53	0.44
13:M:150:MET:C	13:M:153:PRO:HD2	2.43	0.44
6:T:132:THR:O	6:T:146:MET:HA	2.17	0.44
6:T:165:ARG:O	6:T:169:LYS:HG3	2.17	0.44
6:T:191:GLN:HE21	6:T:194:LYS:CE	2.30	0.44
7:U:34:LEU:C	7:U:34:LEU:HD12	2.43	0.44
7:U:115:LEU:HD12	7:U:115:LEU:HA	1.83	0.44
14:b:156:LYS:HG2	14:b:196:LEU:HD11	2.00	0.44
4:D:109:CYS:HB3	4:D:154:GLY:O	2.18	0.44
6:F:133:ILE:HA	6:F:145:TYR:O	2.18	0.44
7:G:74:VAL:HG11	7:G:81:ALA:CB	2.48	0.44
10:J:139:TYR:CZ	10:J:172:MET:HG3	2.53	0.44
14:N:84:GLU:O	14:N:88:GLU:HB2	2.17	0.44
1:O:64:VAL:HG11	1:O:212:ALA:HB3	1.99	0.44
4:R:7:PHE:HB2	5:S:20:GLN:OE1	2.18	0.44
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.43	0.44
14:b:55:ILE:O	14:b:59:VAL:HG23	2.18	0.44
14:b:175:MET:HE3	14:b:188:PHE:CD2	2.53	0.44
9:I:50:LEU:HG	9:I:52:ILE:CD1	2.47	0.44
12:L:174:TYR:CD1	12:L:175:LEU:N	2.86	0.44
2:P:139:TYR:CG	2:P:224:VAL:HG21	2.52	0.44
9:W:20:VAL:CG1	9:W:118:PRO:HB3	2.48	0.44
10:X:53:THR:HG23	10:X:54:VAL:HG23	2.00	0.44
13:a:54:SER:OG	13:a:113:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:PHE:N	2:B:229:PHE:HD2	2.16	0.43
3:C:27:ARG:HB2	3:C:27:ARG:CZ	2.48	0.43
3:C:131:THR:O	3:C:147:GLN:HA	2.18	0.43
6:F:41:GLY:HA3	6:F:215:CYS:O	2.17	0.43
7:G:34:LEU:C	7:G:34:LEU:HD12	2.43	0.43
9:I:104:VAL:HG23	9:I:106:PRO:HD3	2.00	0.43
14:N:107:LYS:HG2	14:N:108:GLY:N	2.33	0.43
1:O:205:ASN:HA	1:O:247:LEU:CD1	2.48	0.43
5:S:1:PHE:O	5:S:2:ARG:C	2.60	0.43
5:S:35:VAL:HG12	5:S:36:GLY:N	2.32	0.43
5:S:86:TYR:CD1	5:S:114:LYS:HD2	2.53	0.43
2:P:65:LEU:HD12	2:P:75:ALA:HA	2.00	0.43
5:S:216:GLY:O	5:S:217:LYS:C	2.61	0.43
6:T:105:ILE:N	6:T:106:PRO:CD	2.82	0.43
7:U:78:ILE:N	7:U:79:PRO:HD2	2.33	0.43
12:Z:51:VAL:CG2	12:Z:112:ALA:HB3	2.48	0.43
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	2.01	0.43
12:Z:208:THR:C	12:Z:210:ASP:N	2.76	0.43
13:a:104:ARG:HG3	13:a:105:SER:N	2.32	0.43
13:a:129:TYR:O	13:a:136:THR:HA	2.17	0.43
13:a:161:ARG:CG	13:a:161:ARG:NH1	2.81	0.43
14:b:107:LYS:HG2	14:b:108:GLY:H	1.82	0.43
1:A:234:ARG:HG2	1:A:234:ARG:NH1	2.33	0.43
1:A:248:GLU:C	1:A:250:LEU:N	2.75	0.43
2:B:120:GLY:C	2:B:122:THR:N	2.77	0.43
2:B:182:ASP:O	2:B:183:MET:C	2.61	0.43
3:C:170:ARG:O	3:C:174:GLU:HG3	2.18	0.43
6:F:32:THR:CG2	6:F:47:GLU:OE2	2.66	0.43
14:N:175:MET:HE3	14:N:188:PHE:CD2	2.53	0.43
2:P:17:ARG:HG2	2:P:17:ARG:NH1	2.33	0.43
2:P:60:THR:HG22	2:P:60:THR:O	2.19	0.43
4:R:51:LEU:HD13	4:R:51:LEU:C	2.43	0.43
6:T:36:ILE:HD12	6:T:192:ALA:HB2	2.00	0.43
6:T:178:HIS:O	6:T:179:HIS:CG	2.72	0.43
7:U:174:GLU:O	7:U:178:LYS:HG3	2.17	0.43
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.53	0.43
12:Z:28:ARG:NE	12:Z:200:ASP:OD2	2.36	0.43
12:Z:208:THR:C	12:Z:210:ASP:H	2.26	0.43
1:A:94:HIS:CD2	8:H:61:SER:OG	2.70	0.43
2:B:119:GLN:NE2	16:B:310:HOH:O	2.50	0.43
3:C:40:VAL:HG22	3:C:143:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ARG:O	3:C:165:ASN:HB2	2.19	0.43
4:D:161:ALA:HB3	5:E:55:LEU:HD23	2.00	0.43
6:F:138:ASP:OD2	6:F:138:ASP:C	2.61	0.43
9:I:68:TYR:C	9:I:68:TYR:CD1	2.96	0.43
2:P:159:TRP:CD2	2:P:162:ILE:HD13	2.54	0.43
3:Q:225:GLU:OE1	3:Q:225:GLU:N	2.50	0.43
6:T:31:THR:CG2	6:T:32:THR:N	2.82	0.43
6:T:123:ASN:C	6:T:123:ASN:ND2	2.76	0.43
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.53	0.43
10:X:118:GLN:NE2	10:X:132:ALA:O	2.52	0.43
10:X:192:VAL:C	10:X:194:ASP:H	2.27	0.43
12:Z:85:SER:HB2	12:Z:87:ASN:OD1	2.19	0.43
12:Z:103:PHE:N	12:Z:104:PRO:CD	2.80	0.43
12:Z:126:ASP:HB2	12:Z:130:SER:N	2.31	0.43
2:B:35:ILE:HG12	2:B:196:LEU:HD21	2.00	0.43
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.00	0.43
6:F:201:GLU:O	6:F:204:LYS:HD2	2.18	0.43
7:G:237:VAL:O	7:G:240:ALA:HB3	2.19	0.43
13:M:151:ALA:O	13:M:152:ASN:C	2.62	0.43
13:M:161:ARG:CG	13:M:161:ARG:NH1	2.81	0.43
3:Q:69:VAL:HG13	3:Q:104:VAL:HG22	2.00	0.43
3:Q:155:SER:CB	4:R:51:LEU:HD21	2.47	0.43
3:Q:214:LYS:HD2	3:Q:218:ASP:OD1	2.19	0.43
4:R:214:ILE:HA	4:R:219:GLY:O	2.19	0.43
5:S:167:ALA:CB	5:S:195:ALA:O	2.67	0.43
5:S:174:THR:O	5:S:177:THR:HB	2.18	0.43
7:U:241:GLU:O	7:U:242:GLN:CB	2.65	0.43
3:C:214:LYS:HD2	3:C:218:ASP:OD1	2.19	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
5:E:174:THR:O	5:E:177:THR:HB	2.18	0.43
8:H:22:GLN:HG3	15:c:2:THR:HG22	2.01	0.43
9:I:69:LYS:NZ	16:I:324:HOH:O	2.51	0.43
12:L:201:GLY:C	12:L:219:LEU:HD12	2.44	0.43
2:P:189:ILE:HG23	2:P:212:PHE:CE2	2.54	0.43
4:R:73:LEU:HD12	4:R:131:GLY:HA3	2.00	0.43
9:W:123:PHE:HA	9:W:128:CYS:O	2.19	0.43
10:X:4:ILE:HD13	10:X:4:ILE:HA	1.91	0.43
3:C:160:GLN:CA	3:C:160:GLN:NE2	2.78	0.43
8:H:156:SER:O	8:H:160:GLN:HG3	2.19	0.43
1:O:28:VAL:HG11	1:O:133:SER:HB2	2.01	0.43
1:O:222:LEU:HD23	1:O:224:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:234:GLU:O	4:R:238:LYS:HG3	2.19	0.43
6:T:133:ILE:HA	6:T:145:TYR:O	2.19	0.43
7:U:12:PRO:HD3	16:U:328:HOH:O	2.19	0.43
9:W:41:LYS:O	9:W:51:GLY:HA2	2.19	0.43
10:X:149:ARG:HG2	10:X:149:ARG:NH1	2.34	0.43
12:Z:13:LEU:O	12:Z:23:LEU:HD23	2.18	0.43
14:b:14:LEU:HD11	14:b:100:ALA:HB3	2.00	0.43
1:A:35:LEU:C	1:A:35:LEU:HD12	2.44	0.43
6:F:95:PHE:CD2	6:F:103:ILE:HD12	2.54	0.43
9:I:76:LYS:NZ	16:I:361:HOH:O	2.52	0.43
13:M:104:ARG:HG3	13:M:105:SER:N	2.32	0.43
2:P:140:ASP:OD2	2:P:146:GLN:NE2	2.47	0.43
4:R:159:TYR:CD2	4:R:162:LYS:HD3	2.54	0.43
7:U:68:ARG:NH1	7:U:68:ARG:HB2	2.33	0.43
1:A:145:PHE:HD1	16:A:306:HOH:O	2.01	0.43
4:D:214:ILE:HA	4:D:219:GLY:O	2.19	0.43
4:D:236:LYS:HE2	4:D:236:LYS:HB3	1.77	0.43
5:E:1:PHE:O	5:E:2:ARG:C	2.61	0.43
11:K:75:SER:HB2	11:K:108:GLU:OE2	2.18	0.43
11:K:169:ALA:HB1	9:W:178:ALA:O	2.18	0.43
13:M:201:ASP:HB3	13:M:204:THR:OG1	2.18	0.43
14:N:44:CYS:HB2	14:N:98:ILE:HB	2.00	0.43
3:Q:7:SER:O	4:R:128:ARG:HD3	2.18	0.43
8:V:40:LYS:HE2	8:V:183:ASP:HA	2.00	0.43
11:Y:106:ARG:HG2	11:Y:106:ARG:NH1	2.34	0.43
14:b:13:ILE:HD12	14:b:151:THR:CG2	2.49	0.43
1:A:231:LYS:HB2	16:A:347:HOH:O	2.19	0.43
3:C:101:PRO:HG2	3:C:138:PRO:HG3	2.01	0.43
8:H:38:SER:OG	8:H:41:ILE:HD13	2.19	0.43
8:H:104:ASP:C	8:H:106:THR:N	2.77	0.43
9:I:26:LEU:CD2	9:I:40:GLU:HG2	2.49	0.43
10:J:130:TYR:CD2	10:J:144:LEU:HD13	2.54	0.43
12:L:57:PHE:CZ	12:L:59:ALA:HB3	2.54	0.43
1:O:234:ARG:HG2	1:O:234:ARG:NH1	2.33	0.43
1:O:250:LEU:C	1:O:250:LEU:HD13	2.43	0.43
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.83	0.43
6:T:71:GLY:O	6:T:134:PHE:HA	2.19	0.43
8:V:10:ASN:O	8:V:179:GLU:HG3	2.19	0.43
10:X:8:ARG:HG2	10:X:8:ARG:NH1	2.34	0.43
14:b:44:CYS:HB2	14:b:98:ILE:HB	2.01	0.43
4:D:59:ILE:HD12	4:D:210:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:165:ARG:HE	6:F:165:ARG:HB3	1.50	0.42
10:J:118:GLN:NE2	10:J:132:ALA:O	2.52	0.42
12:L:213:ARG:CB	12:L:213:ARG:HH11	2.32	0.42
2:P:24:ALA:O	2:P:27:SER:HB3	2.19	0.42
2:P:41:ASP:OD2	2:P:41:ASP:N	2.49	0.42
2:P:229:PHE:N	2:P:229:PHE:HD2	2.17	0.42
4:R:31:GLY:O	4:R:161:ALA:HA	2.19	0.42
6:T:172:LEU:HD22	6:T:195:ILE:HD13	2.01	0.42
7:U:232:ILE:O	7:U:235:ARG:N	2.51	0.42
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.19	0.42
10:X:78:GLN:NE2	10:X:78:GLN:C	2.77	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.00	0.42
2:B:135:ILE:HD11	2:B:164:VAL:HG22	2.01	0.42
2:B:240:LYS:C	2:B:242:GLY:N	2.76	0.42
4:D:60:VAL:HG21	4:D:81:ILE:CD1	2.47	0.42
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.00	0.42
11:K:38:ASN:C	11:K:38:ASN:OD1	2.61	0.42
11:K:116:ASP:OD1	11:K:116:ASP:C	2.63	0.42
12:L:220:LYS:HG3	16:L:352:HOH:O	2.19	0.42
13:M:11:VAL:O	13:M:143:ALA:HA	2.19	0.42
13:M:65:ARG:CD	16:M:336:HOH:O	2.67	0.42
13:M:78:ASN:ND2	13:M:81:ALA:HA	2.35	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
11:Y:15:ALA:C	11:Y:161:ILE:HD11	2.45	0.42
12:Z:174:TYR:CD1	12:Z:175:LEU:N	2.88	0.42
14:b:146:MET:HE2	14:b:150:GLU:C	2.44	0.42
5:E:181:ILE:HG21	5:E:187:GLU:CB	2.47	0.42
6:F:168:ALA:C	6:F:172:LEU:HD23	2.44	0.42
8:H:10:ASN:O	8:H:179:GLU:HG3	2.19	0.42
8:H:148:LYS:HD3	16:H:346:HOH:O	2.19	0.42
12:L:3:ASN:ND2	12:L:3:ASN:C	2.75	0.42
12:L:208:THR:C	12:L:210:ASP:H	2.28	0.42
13:M:74:ASN:HB3	16:M:318:HOH:O	2.19	0.42
13:M:168:THR:HA	16:M:359:HOH:O	2.19	0.42
1:O:226:GLY:HA3	8:V:186:TYR:HB3	2.01	0.42
2:P:120:GLY:C	2:P:122:THR:N	2.76	0.42
3:Q:95:ARG:HH11	3:Q:101:PRO:HB3	1.82	0.42
3:Q:225:GLU:O	3:Q:229:GLN:HG3	2.19	0.42
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.01	0.42
12:Z:89:ALA:O	12:Z:93:ILE:HG12	2.19	0.42
1:A:203:GLU:HA	1:A:203:GLU:OE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:TYR:HB2	2:B:148:TYR:HB2	2.01	0.42
6:F:237:ASP:O	6:F:238:PHE:C	2.61	0.42
12:L:51:VAL:HG23	12:L:112:ALA:HB3	2.01	0.42
13:M:213:GLN:HE21	13:M:213:GLN:HB3	1.48	0.42
3:Q:27:ARG:NH1	3:Q:27:ARG:CB	2.83	0.42
4:R:140:ASP:OD2	4:R:140:ASP:C	2.62	0.42
5:S:131:LEU:HD12	5:S:146:PHE:CD2	2.54	0.42
7:U:228:SER:O	7:U:229:ALA:C	2.63	0.42
14:b:66:TYR:CE2	14:b:73:PRO:HB3	2.55	0.42
2:B:17:ARG:HG2	2:B:17:ARG:HH11	1.84	0.42
3:C:225:GLU:O	3:C:229:GLN:HG3	2.18	0.42
4:D:54:ASP:OD2	4:D:54:ASP:N	2.48	0.42
4:D:73:LEU:HD12	4:D:131:GLY:HA3	2.02	0.42
2:P:99:LYS:HZ3	10:X:86:GLN:NE2	2.16	0.42
3:Q:164:ARG:O	3:Q:165:ASN:HB2	2.19	0.42
4:R:159:TYR:HA	5:S:55:LEU:O	2.20	0.42
6:T:34:ILE:HG22	6:T:160:ALA:HB1	1.96	0.42
12:Z:98:TYR:CE2	12:Z:101:ARG:HD3	2.55	0.42
13:a:21:ILE:HG12	13:a:199:ILE:HG23	2.01	0.42
1:A:28:VAL:HG11	1:A:133:SER:HB2	2.02	0.42
2:B:65:LEU:HD12	2:B:75:ALA:HA	2.01	0.42
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.54	0.42
3:C:107:LEU:O	3:C:107:LEU:HD13	2.19	0.42
3:C:225:GLU:H	3:C:225:GLU:CD	2.28	0.42
4:D:194:LYS:HE2	4:D:198:GLN:OE1	2.20	0.42
5:E:73:LEU:C	5:E:73:LEU:HD12	2.44	0.42
6:F:71:GLY:O	6:F:134:PHE:HA	2.19	0.42
6:F:172:LEU:HD22	6:F:195:ILE:HD13	2.02	0.42
7:G:210:SER:O	7:G:236:LEU:HD21	2.19	0.42
9:I:11:VAL:HG22	9:I:24:CYS:HB3	2.01	0.42
1:O:36:GLY:HA2	1:O:44:VAL:O	2.20	0.42
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.20	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
4:R:194:LYS:HE2	4:R:198:GLN:OE1	2.19	0.42
11:Y:12:ILE:HD13	11:Y:112:ILE:CD1	2.50	0.42
12:Z:3:ASN:HD22	12:Z:4:PRO:N	2.17	0.42
13:a:25:ASP:OD2	13:a:25:ASP:C	2.63	0.42
1:A:250:LEU:HD13	1:A:250:LEU:C	2.45	0.42
2:B:1:GLY:HA3	5:E:122:TYR:CE1	2.55	0.42
2:B:180:LYS:O	2:B:183:MET:HG3	2.19	0.42
2:B:234:ILE:O	2:B:238:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:NH1	7:G:68:ARG:HB2	2.33	0.42
12:L:38:ARG:NH1	12:L:221:ARG:HB3	2.35	0.42
14:N:26:ILE:HB	13:a:187:ARG:HA	2.01	0.42
1:O:94:HIS:CD2	8:V:61:SER:OG	2.72	0.42
3:Q:131:THR:O	3:Q:147:GLN:HA	2.19	0.42
4:R:37:GLY:HA2	4:R:145:TYR:CD1	2.54	0.42
8:V:22:GLN:HG3	15:e:2:THR:HG22	2.01	0.42
11:Y:116:ASP:C	11:Y:116:ASP:OD1	2.61	0.42
14:b:14:LEU:HD12	14:b:14:LEU:N	2.34	0.42
1:A:66:LEU:C	1:A:66:LEU:CD2	2.93	0.42
1:A:120:GLU:C	1:A:122:THR:H	2.27	0.42
13:M:54:SER:OG	13:M:113:ALA:HB3	2.20	0.42
3:Q:101:PRO:HG2	3:Q:138:PRO:HG3	1.99	0.42
6:T:168:ALA:C	6:T:172:LEU:HD23	2.45	0.42
10:X:129:PRO:HB2	10:X:130:TYR:CD1	2.55	0.42
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.93	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
3:C:222:LEU:N	3:C:222:LEU:CD1	2.83	0.42
5:E:49:LYS:HB3	5:E:58:TYR:HB3	2.01	0.42
6:F:34:ILE:HG22	6:F:160:ALA:HB1	1.99	0.42
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.20	0.42
10:J:78:GLN:NE2	10:J:78:GLN:C	2.78	0.42
12:L:208:THR:C	12:L:210:ASP:N	2.77	0.42
13:M:25:ASP:HA	13:M:195:PHE:CB	2.50	0.42
2:P:36:GLY:O	2:P:161:ALA:HA	2.20	0.42
2:P:57:GLU:OE1	2:P:57:GLU:HA	2.20	0.42
2:P:105:ILE:HG22	16:P:309:HOH:O	2.19	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
4:R:193:LEU:HD12	4:R:193:LEU:HA	1.88	0.42
5:S:33:VAL:HG22	5:S:34:THR:N	2.35	0.42
5:S:61:LYS:O	5:S:72:SER:HA	2.20	0.42
6:T:32:THR:CG2	6:T:47:GLU:OE2	2.67	0.42
6:T:237:ASP:C	6:T:239:ALA:N	2.76	0.42
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.02	0.42
7:U:224:PHE:CD1	7:U:224:PHE:C	2.97	0.42
9:W:37:ASN:HD22	9:W:37:ASN:C	2.28	0.42
13:a:78:ASN:ND2	13:a:81:ALA:HA	2.35	0.42
2:B:189:ILE:HG23	2:B:212:PHE:CE2	2.55	0.42
4:D:140:ASP:OD2	4:D:140:ASP:C	2.62	0.42
5:E:106:ARG:HG2	5:E:106:ARG:HH11	1.84	0.42
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.19	0.42
9:I:37:ASN:C	9:I:37:ASN:HD22	2.28	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
10:J:18:SER:HB2	10:J:176:PHE:HB2	2.02	0.42
14:N:139:ASP:HB3	14:b:161:GLN:NE2	2.35	0.42
1:O:120:GLU:C	1:O:122:THR:H	2.27	0.42
2:P:182:ASP:O	2:P:183:MET:C	2.62	0.42
2:P:239:VAL:HG12	2:P:240:LYS:N	2.35	0.42
4:R:85:ARG:O	4:R:89:VAL:HG23	2.20	0.42
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.01	0.42
11:Y:9:GLN:HE21	11:Y:9:GLN:HB3	1.70	0.42
2:B:140:ASP:OD2	2:B:146:GLN:NE2	2.45	0.41
5:E:216:GLY:O	5:E:217:LYS:C	2.63	0.41
6:F:165:ARG:O	6:F:169:LYS:HG3	2.20	0.41
12:L:213:ARG:NH1	12:L:213:ARG:HB3	2.35	0.41
2:P:35:ILE:HG12	2:P:196:LEU:HD21	2.01	0.41
3:Q:57:ILE:H	3:Q:57:ILE:HD13	1.85	0.41
9:W:137:VAL:HG11	9:W:145:LEU:HB3	2.00	0.41
10:X:194:ASP:O	10:X:198:GLN:HB2	2.18	0.41
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.56	0.41
6:F:214:TRP:N	6:F:214:TRP:CD1	2.88	0.41
7:G:78:ILE:N	7:G:79:PRO:HD2	2.35	0.41
7:G:103:MET:HE3	7:G:108:LEU:HD13	2.01	0.41
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.20	0.41
12:L:85:SER:HB2	12:L:87:ASN:OD1	2.20	0.41
12:L:159:GLN:HG2	8:V:209:THR:CG2	2.48	0.41
13:M:162:GLU:O	13:M:165:ILE:HG13	2.20	0.41
2:P:234:ILE:O	2:P:238:LEU:HB2	2.20	0.41
4:R:24:LYS:O	4:R:166:SER:HA	2.20	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
5:S:49:LYS:HB3	5:S:58:TYR:HB3	2.01	0.41
5:S:181:ILE:HG21	5:S:187:GLU:CB	2.49	0.41
7:U:230:GLU:HG2	16:U:356:HOH:O	2.19	0.41
9:W:104:VAL:HG23	9:W:106:PRO:HD3	2.02	0.41
13:a:1:THR:N	13:a:107:MET:O	2.47	0.41
1:A:89:SER:O	1:A:92:VAL:HG12	2.21	0.41
3:C:69:VAL:HG13	3:C:104:VAL:HG22	2.01	0.41
4:D:169:GLU:OE1	4:D:169:GLU:N	2.53	0.41
5:E:81:ARG:O	5:E:85:ASN:HB2	2.21	0.41
6:F:31:THR:CG2	6:F:32:THR:N	2.83	0.41
6:F:112:LEU:O	6:F:116:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:166:GLN:NE2	7:G:167:GLN:N	2.67	0.41
7:G:187:GLU:HG2	7:G:192:LYS:HB3	2.01	0.41
10:J:192:VAL:C	10:J:194:ASP:H	2.28	0.41
13:M:187:ARG:HA	14:b:26:ILE:HB	2.01	0.41
14:N:159:LEU:O	14:N:163:ILE:CD1	2.68	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CE1	2.54	0.41
6:T:200:HIS:O	6:T:200:HIS:CG	2.73	0.41
7:U:231:ASN:N	7:U:231:ASN:HD22	2.17	0.41
9:W:26:LEU:CD2	9:W:40:GLU:HG2	2.49	0.41
12:Z:20:PHE:CE1	12:Z:177:VAL:HA	2.55	0.41
13:a:132:LEU:HD23	13:a:132:LEU:N	2.35	0.41
14:b:159:LEU:O	14:b:163:ILE:CD1	2.68	0.41
2:B:95:GLN:NE2	16:B:307:HOH:O	2.52	0.41
4:D:85:ARG:HD2	16:D:304:HOH:O	2.20	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.41
9:I:30:SER:O	9:I:31:GLN:HB2	2.20	0.41
10:J:46:PHE:HB3	10:J:102:VAL:HG12	2.01	0.41
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.41
11:K:52:CYS:O	11:K:56:GLU:HB2	2.20	0.41
1:O:89:SER:O	1:O:92:VAL:HG12	2.20	0.41
5:S:84:SER:O	5:S:88:ARG:HG3	2.21	0.41
9:W:28:LEU:HD13	9:W:28:LEU:C	2.45	0.41
13:a:201:ASP:HB3	13:a:204:THR:OG1	2.21	0.41
14:b:15:GLY:HA2	14:b:174:ARG:O	2.21	0.41
14:b:107:LYS:HG2	14:b:108:GLY:N	2.35	0.41
2:B:18:LEU:O	2:B:22:GLU:HG2	2.21	0.41
3:C:57:ILE:HG12	3:C:58:THR:N	2.35	0.41
4:D:51:LEU:C	4:D:51:LEU:HD13	2.45	0.41
5:E:33:VAL:HG22	5:E:34:THR:N	2.36	0.41
6:F:191:GLN:HE21	6:F:194:LYS:CE	2.33	0.41
7:G:49:LYS:O	7:G:51:PRO:HD3	2.21	0.41
11:K:8:PHE:HA	11:K:146:TRP:CE3	2.56	0.41
3:Q:107:LEU:O	3:Q:111:VAL:HG23	2.20	0.41
5:S:106:ARG:HG2	5:S:106:ARG:HH11	1.85	0.41
6:T:115:TYR:O	6:T:118:ALA:HB3	2.20	0.41
8:V:144:GLN:O	8:V:145:ASP:HB2	2.20	0.41
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.02	0.41
14:b:143:ARG:NH2	16:b:238:HOH:O	2.54	0.41
3:C:20:TYR:N	3:C:20:TYR:CD1	2.89	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41
10:J:96:ARG:HH11	10:J:96:ARG:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:HE2	10:X:173:PRO:C	2.46	0.41
12:L:13:LEU:O	12:L:23:LEU:HD23	2.21	0.41
13:M:14:MET:HE3	13:M:159:VAL:CG2	2.51	0.41
2:P:1:GLY:HA3	5:S:122:TYR:CE1	2.55	0.41
6:T:41:GLY:CA	6:T:215:CYS:O	2.68	0.41
7:U:179:LYS:HE3	7:U:179:LYS:HB2	1.76	0.41
10:X:96:ARG:HG2	10:X:96:ARG:HH11	1.85	0.41
1:A:30:GLN:HE21	1:A:30:GLN:CA	2.25	0.41
2:B:6:ASP:OD1	3:C:4:ARG:HG3	2.20	0.41
3:C:170:ARG:HB2	3:C:170:ARG:NH1	2.35	0.41
5:E:230:ALA:C	5:E:232:TYR:H	2.28	0.41
6:F:200:HIS:O	6:F:200:HIS:CG	2.73	0.41
7:G:19:VAL:O	7:G:23:PHE:HD2	2.04	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.02	0.41
7:G:198:ILE:O	7:G:202:ILE:HG13	2.20	0.41
9:I:62:LEU:HD21	9:I:102:TYR:CD1	2.56	0.41
9:I:122:GLY:O	9:I:130:ASP:HB3	2.21	0.41
11:K:106:ARG:NH1	11:K:106:ARG:HG2	2.36	0.41
12:L:10:GLY:HA3	12:L:42:LYS:HZ1	1.85	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
2:P:136:TYR:HB2	2:P:148:TYR:HB2	2.02	0.41
3:Q:116:GLN:NE2	3:Q:116:GLN:C	2.78	0.41
6:T:103:ILE:HA	6:T:104:PRO:HD3	1.92	0.41
16:T:316:HOH:O	7:U:87:ARG:HB2	2.19	0.41
7:U:93:ALA:CB	14:b:65:LEU:HD13	2.51	0.41
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.21	0.41
10:X:149:ARG:HA	10:X:150:PRO:HD3	1.93	0.41
5:E:9:THR:HG21	5:E:126:PRO:HG3	2.03	0.41
5:E:178:PHE:C	5:E:180:LYS:N	2.78	0.41
6:F:105:ILE:CG2	6:F:143:HIS:HB2	2.48	0.41
7:G:179:LYS:HB2	7:G:179:LYS:HE3	1.76	0.41
8:H:144:GLN:O	8:H:145:ASP:HB2	2.20	0.41
9:I:41:LYS:O	9:I:51:GLY:HA2	2.21	0.41
10:J:23:ARG:HD3	10:J:23:ARG:HA	1.95	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.21	0.41
11:K:199:LYS:N	16:K:338:HOH:O	2.53	0.41
12:L:31:THR:O	12:L:32:ASP:HB2	2.21	0.41
12:L:126:ASP:HB2	12:L:130:SER:N	2.30	0.41
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.01	0.41
1:O:66:LEU:C	1:O:66:LEU:CD2	2.93	0.41
2:P:128:ARG:HA	2:P:129:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:170:ARG:NH1	3:Q:170:ARG:HB2	2.35	0.41
5:S:99:ASN:HB2	13:a:94:GLU:CG	2.47	0.41
6:T:28:GLU:HB3	6:T:165:ARG:NH2	2.36	0.41
7:U:3:TYR:C	7:U:5:ARG:N	2.78	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.41
1:A:36:GLY:HA2	1:A:44:VAL:O	2.21	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.41
2:B:237:ILE:O	2:B:237:ILE:HG13	2.21	0.41
4:D:37:GLY:HA2	4:D:145:TYR:CD1	2.56	0.41
4:D:82:GLU:OE1	11:K:69:ARG:HD2	2.21	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.41
4:D:159:TYR:CD2	4:D:162:LYS:HD3	2.53	0.41
6:F:41:GLY:CA	6:F:215:CYS:O	2.69	0.41
6:F:46:VAL:HG22	6:F:47:GLU:N	2.35	0.41
6:F:237:ASP:C	6:F:239:ALA:N	2.78	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.55	0.41
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.02	0.41
8:H:40:LYS:HE2	8:H:183:ASP:HA	2.03	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
9:I:37:ASN:HD22	9:I:38:LYS:HG3	1.84	0.41
9:I:137:VAL:HG11	9:I:145:LEU:HB3	2.03	0.41
11:K:8:PHE:O	11:K:9:GLN:C	2.64	0.41
11:K:13:ILE:HG13	11:K:153:ALA:HB1	2.03	0.41
12:L:3:ASN:HD22	12:L:4:PRO:N	2.19	0.41
14:N:82:PHE:HB3	14:N:113:ILE:HD12	2.02	0.41
2:P:38:MET:HE2	2:P:145:TYR:O	2.20	0.41
3:Q:9:PHE:CE1	3:Q:15:ILE:HD11	2.56	0.41
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	2.03	0.41
3:Q:225:GLU:H	3:Q:225:GLU:CD	2.29	0.41
4:R:168:SER:O	4:R:172:GLN:HB2	2.21	0.41
4:R:169:GLU:OE1	4:R:169:GLU:N	2.54	0.41
7:U:49:LYS:O	7:U:51:PRO:HD3	2.21	0.41
8:V:156:SER:HB3	16:V:318:HOH:O	2.21	0.41
9:W:124:ASP:HB3	15:e:2:THR:HG23	2.02	0.41
9:W:154:GLU:O	9:W:157:LEU:HG	2.21	0.41
11:Y:106:ARG:HG2	11:Y:106:ARG:HH11	1.84	0.41
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.56	0.41
3:C:157:TRP:NE1	4:D:51:LEU:HD23	2.35	0.41
10:J:150:PRO:HG2	11:Y:208:ASN:HD21	1.86	0.41
3:Q:110:TYR:O	3:Q:114:VAL:HG23	2.20	0.41
4:R:155:THR:HG22	5:S:77:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:105:ILE:CG2	6:T:143:HIS:HB2	2.49	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
8:V:104:ASP:C	8:V:106:THR:N	2.79	0.41
11:Y:38:ASN:C	11:Y:38:ASN:OD1	2.63	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.03	0.41
12:Z:108:HIS:HE1	12:Z:124:SER:HB2	1.85	0.41
2:B:36:GLY:O	2:B:161:ALA:HA	2.21	0.40
2:B:41:ASP:OD2	2:B:41:ASP:N	2.52	0.40
6:F:178:HIS:O	6:F:179:HIS:CG	2.74	0.40
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.62	0.40
9:I:37:ASN:ND2	9:I:37:ASN:H	2.19	0.40
1:O:35:LEU:C	1:O:35:LEU:HD12	2.46	0.40
1:O:235:PHE:CD2	1:O:235:PHE:C	2.98	0.40
6:T:214:TRP:CH2	6:T:219:GLU:HB3	2.56	0.40
7:U:210:SER:O	7:U:236:LEU:HD21	2.21	0.40
12:Z:49:ASN:HD22	12:Z:49:ASN:HA	1.73	0.40
13:a:151:ALA:O	13:a:152:ASN:C	2.64	0.40
1:A:174:PHE:O	1:A:178:ARG:HG2	2.21	0.40
3:C:57:ILE:H	3:C:57:ILE:HD13	1.86	0.40
3:C:178:ASP:OD1	3:C:180:LYS:HB2	2.21	0.40
5:E:172:GLU:CD	6:F:52:SER:HB2	2.47	0.40
6:F:153:TYR:CD1	6:F:153:TYR:C	2.98	0.40
9:I:65:MET:O	9:I:68:TYR:HB3	2.21	0.40
10:J:26:SER:HB2	11:K:133:GLN:NE2	2.36	0.40
10:J:173:PRO:C	10:X:174:MET:HE2	2.45	0.40
13:M:129:TYR:O	13:M:136:THR:HA	2.20	0.40
13:M:169:THR:HG23	16:M:359:HOH:O	2.21	0.40
1:O:211:LEU:HD23	1:O:211:LEU:C	2.46	0.40
5:S:207:VAL:HG22	5:S:226:GLY:C	2.45	0.40
5:S:226:GLY:O	5:S:227:GLU:C	2.65	0.40
6:T:171:GLU:OE1	6:T:198:LEU:HD23	2.21	0.40
8:V:78:SER:O	8:V:82:MET:HG3	2.21	0.40
13:a:88:GLU:HB2	13:a:91:TYR:CD2	2.56	0.40
14:b:82:PHE:HB3	14:b:113:ILE:HD12	2.03	0.40
2:B:119:GLN:NE2	2:B:119:GLN:C	2.80	0.40
4:D:4:VAL:HG23	4:D:116:GLY:HA2	2.03	0.40
5:E:178:PHE:C	5:E:178:PHE:CD1	2.99	0.40
6:F:17:ASN:ND2	6:F:20:VAL:HG23	2.36	0.40
6:F:83:HIS:CD2	6:F:128:PHE:HE2	2.37	0.40
10:J:60:ILE:HD13	10:J:60:ILE:HA	1.94	0.40
12:L:5:TYR:CE2	12:L:106:TYR:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:119:GLN:NE2	2:P:119:GLN:C	2.80	0.40
4:R:109:CYS:HB3	4:R:154:GLY:O	2.21	0.40
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.62	0.40
5:S:85:ASN:O	5:S:89:GLN:HG3	2.21	0.40
6:T:214:TRP:CD1	6:T:214:TRP:N	2.87	0.40
10:X:46:PHE:HB3	10:X:102:VAL:HG12	2.03	0.40
11:Y:8:PHE:HA	11:Y:146:TRP:CE3	2.56	0.40
12:Z:30:ILE:C	12:Z:30:ILE:CD1	2.91	0.40
1:A:158:PRO:HG2	2:B:57:GLU:HB3	2.03	0.40
2:B:172:GLN:HG2	3:C:50:LEU:HD12	2.04	0.40
2:B:223:GLU:CG	2:B:224:VAL:N	2.85	0.40
3:C:66:ASP:OD1	3:C:95:ARG:NH1	2.54	0.40
5:E:206:THR:H	5:E:209:ASN:HD22	1.69	0.40
6:F:115:TYR:O	6:F:118:ALA:HB3	2.21	0.40
6:F:176:VAL:HG21	7:G:54:LEU:HD23	2.04	0.40
7:G:87:ARG:CZ	7:G:115:LEU:HD21	2.52	0.40
14:N:15:GLY:HA2	14:N:174:ARG:O	2.22	0.40
3:Q:66:ASP:OD1	3:Q:95:ARG:NH1	2.55	0.40
6:T:105:ILE:N	6:T:105:ILE:CD1	2.84	0.40
6:T:186:ARG:HH11	6:T:186:ARG:CG	2.34	0.40
7:U:87:ARG:CZ	7:U:115:LEU:HD21	2.52	0.40
8:V:18:THR:CB	8:V:30:ASN:HD22	2.34	0.40
10:X:18:SER:HB2	10:X:176:PHE:HB2	2.03	0.40
12:Z:5:TYR:CE2	12:Z:106:TYR:HB2	2.57	0.40
12:Z:80:ASN:HD22	12:Z:80:ASN:HA	1.63	0.40
1:A:235:PHE:CD2	1:A:235:PHE:C	2.99	0.40
5:E:167:ALA:CB	5:E:195:ALA:O	2.69	0.40
5:E:174:THR:O	5:E:175:LEU:C	2.63	0.40
5:E:226:GLY:O	5:E:227:GLU:C	2.64	0.40
6:F:123:ASN:HD22	6:F:123:ASN:N	2.18	0.40
7:G:224:PHE:CD1	7:G:224:PHE:C	2.99	0.40
12:L:20:PHE:CE1	12:L:177:VAL:HA	2.57	0.40
12:L:165:ASN:O	12:L:167:LYS:HG2	2.21	0.40
3:Q:197:LEU:HD13	3:Q:208:ILE:HG23	2.03	0.40
3:Q:213:VAL:HG13	3:Q:213:VAL:O	2.21	0.40
4:R:38:VAL:HG11	4:R:137:ALA:HB1	2.04	0.40
4:R:59:ILE:HD12	4:R:210:GLN:HE21	1.86	0.40
11:Y:52:CYS:O	11:Y:56:GLU:HB2	2.22	0.40
11:Y:176:ASN:HD22	11:Y:176:ASN:HA	1.69	0.40
12:Z:165:ASN:O	12:Z:167:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	226 (91%)	17 (7%)	5 (2%)	6	21
1	O	248/250 (99%)	226 (91%)	18 (7%)	4 (2%)	7	27
2	B	242/244 (99%)	212 (88%)	24 (10%)	6 (2%)	4	16
2	P	242/244 (99%)	213 (88%)	23 (10%)	6 (2%)	4	16
3	C	239/241 (99%)	218 (91%)	15 (6%)	6 (2%)	4	16
3	Q	239/241 (99%)	217 (91%)	16 (7%)	6 (2%)	4	16
4	D	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	5	20
4	R	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	5	20
5	E	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	2	8
5	S	231/233 (99%)	204 (88%)	20 (9%)	7 (3%)	3	12
6	F	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	16	44
6	T	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	16	44
7	G	241/243 (99%)	223 (92%)	15 (6%)	3 (1%)	10	34
7	U	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	34
8	H	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	14	41
8	V	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	9	30
9	I	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	24	55
9	W	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	24	55
10	J	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	12	38
10	X	196/198 (99%)	182 (93%)	13 (7%)	1 (0%)	24	55
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	55
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	55
12	L	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	24	55
12	Z	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	24	55
13	M	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	14	41
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6312/6368 (99%)	5794 (92%)	432 (7%)	86 (1%)	9	30

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
2	B	51	VAL
2	B	221	ASP
3	C	52	LEU
3	C	203	THR
4	D	122	GLU
5	E	2	ARG
7	G	242	GLN
1	O	53	SER
2	P	51	VAL
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
7	U	242	GLN
2	B	62	THR
2	B	218	GLY
3	C	183	PRO
4	D	181	SER
5	E	175	LEU
5	E	201	ARG
5	E	217	LYS
9	I	191	LYS
10	J	193	ASP
12	L	81	ASP
2	P	62	THR
2	P	218	GLY
3	Q	183	PRO
3	Q	203	THR
4	R	181	SER
5	S	175	LEU
5	S	201	ARG
5	S	217	LYS

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Mol	Chain	Res	Type
6	T	139	LYS
9	W	191	LYS
10	X	193	ASP
12	Z	81	ASP
2	B	183	MET
3	C	202	GLN
4	D	121	GLY
5	E	176	ASP
5	E	221	PHE
6	F	139	LYS
6	F	203	ASN
7	G	51	PRO
1	O	166	LYS
2	P	183	MET
3	Q	202	GLN
4	R	120	SER
4	R	121	GLY
5	S	176	ASP
5	S	221	PHE
6	T	203	ASN
7	U	51	PRO
1	A	2	THR
1	A	166	LYS
1	A	249	ALA
3	C	47	ARG
4	D	120	SER
8	H	105	PRO
10	J	186	LYS
1	O	2	THR
1	O	249	ALA
3	Q	47	ARG
8	V	91	GLN
8	V	105	PRO
1	A	3	ASP
5	E	227	GLU
8	H	91	GLN
13	M	10	SER
13	a	111	TRP
4	D	118	GLY
5	E	231	LYS
7	G	2	GLY
4	R	118	GLY

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Mol	Chain	Res	Type
8	V	9	ASN
13	a	10	SER
5	S	181	ILE
7	U	2	GLY
5	E	181	ILE
11	Y	39	PRO
2	B	243	ILE
3	C	204	GLY
11	K	39	PRO
2	P	243	ILE
3	Q	204	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	199 (95%)	10 (5%)	23	56
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	56
2	B	203/203 (100%)	192 (95%)	11 (5%)	20	51
2	P	203/203 (100%)	192 (95%)	11 (5%)	20	51
3	C	213/213 (100%)	204 (96%)	9 (4%)	26	61
3	Q	213/213 (100%)	204 (96%)	9 (4%)	26	61
4	D	198/198 (100%)	187 (94%)	11 (6%)	19	50
4	R	198/198 (100%)	187 (94%)	11 (6%)	19	50
5	E	192/192 (100%)	182 (95%)	10 (5%)	21	53
5	S	192/192 (100%)	182 (95%)	10 (5%)	21	53
6	F	201/201 (100%)	182 (90%)	19 (10%)	8	26
6	T	201/201 (100%)	182 (90%)	19 (10%)	8	26
7	G	207/207 (100%)	197 (95%)	10 (5%)	23	56
7	U	207/207 (100%)	197 (95%)	10 (5%)	23	56
8	H	181/181 (100%)	173 (96%)	8 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	181/181 (100%)	173 (96%)	8 (4%)	25	59
9	I	172/172 (100%)	165 (96%)	7 (4%)	27	62
9	W	172/172 (100%)	164 (95%)	8 (5%)	23	57
10	J	175/175 (100%)	170 (97%)	5 (3%)	37	73
10	X	175/175 (100%)	170 (97%)	5 (3%)	37	73
11	K	169/169 (100%)	161 (95%)	8 (5%)	23	57
11	Y	169/169 (100%)	161 (95%)	8 (5%)	23	57
12	L	185/185 (100%)	171 (92%)	14 (8%)	12	36
12	Z	185/185 (100%)	173 (94%)	12 (6%)	15	43
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	58
13	a	199/199 (100%)	190 (96%)	9 (4%)	24	58
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	60
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	60
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
All	All	5336/5336 (100%)	5061 (95%)	275 (5%)	21	53

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	29	LYS
1	A	30	GLN
1	A	59	GLU
1	A	66	LEU
1	A	122	THR
1	A	134	LEU
1	A	157	PHE
1	A	178	ARG
1	A	213	ILE
2	B	55	LEU
2	B	65	LEU
2	B	119	GLN
2	B	122	THR

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Mol	Chain	Res	Type
2	B	149	THR
2	B	155	ASN
2	B	157	THR
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
2	B	239	VAL
3	C	4	ARG
3	C	19	GLU
3	C	51	LYS
3	C	55	THR
3	C	57	ILE
3	C	69	VAL
3	C	147	GLN
3	C	160	GLN
3	C	181	GLU
4	D	20	LEU
4	D	40	LEU
4	D	68	CYS
4	D	99	ILE
4	D	102	GLU
4	D	169	GLU
4	D	176	LEU
4	D	182	SER
4	D	183	LEU
4	D	193	LEU
4	D	214	ILE
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	92	ASN
5	E	179	ILE
5	E	197	SER
5	E	198	GLN
5	E	205	LEU
5	E	222	THR
5	E	227	GLU
6	F	7	SER
6	F	32	THR
6	F	39	ASN
6	F	68	ARG
6	F	78	ILE

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Mol	Chain	Res	Type
6	F	94	SER
6	F	101	THR
6	F	103	ILE
6	F	117	GLN
6	F	123	ASN
6	F	131	SER
6	F	165	ARG
6	F	181	GLU
6	F	186	ARG
6	F	196	ILE
6	F	201	GLU
6	F	203	ASN
6	F	221	ASN
6	F	243	ILE
7	G	24	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	120	THR
7	G	166	GLN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	156	SER
8	H	196	ARG
9	I	37	ASN
9	I	52	ILE
9	I	123	PHE
9	I	166	ILE
9	I	171	LEU
9	I	191	LYS
9	I	202	ARG
10	J	69	ILE
10	J	71	GLU
10	J	92	ILE

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Mol	Chain	Res	Type
10	J	174	MET
10	J	189	ILE
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	107	LYS
11	K	147	ASP
11	K	211	ILE
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	52	MET
12	L	70	ASN
12	L	71	SER
12	L	80	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	127	PRO
12	L	132	GLU
12	L	181	ILE
12	L	206	ILE
13	M	37	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	213	GLN
14	N	6	VAL
14	N	36	ARG
14	N	83	LYS
14	N	88	GLU
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
1	O	4	ARG
1	O	29	LYS

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Mol	Chain	Res	Type
1	O	30	GLN
1	O	59	GLU
1	O	66	LEU
1	O	122	THR
1	O	134	LEU
1	O	157	PHE
1	O	178	ARG
1	O	213	ILE
2	P	55	LEU
2	P	65	LEU
2	P	119	GLN
2	P	122	THR
2	P	149	THR
2	P	155	ASN
2	P	157	THR
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
2	P	239	VAL
3	Q	4	ARG
3	Q	19	GLU
3	Q	51	LYS
3	Q	55	THR
3	Q	57	ILE
3	Q	69	VAL
3	Q	147	GLN
3	Q	160	GLN
3	Q	181	GLU
4	R	20	LEU
4	R	40	LEU
4	R	68	CYS
4	R	99	ILE
4	R	102	GLU
4	R	169	GLU
4	R	176	LEU
4	R	182	SER
4	R	183	LEU
4	R	193	LEU
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	71	LEU

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Mol	Chain	Res	Type
5	S	92	ASN
5	S	179	ILE
5	S	197	SER
5	S	198	GLN
5	S	205	LEU
5	S	222	THR
5	S	227	GLU
6	T	7	SER
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	78	ILE
6	T	94	SER
6	T	101	THR
6	T	103	ILE
6	T	117	GLN
6	T	123	ASN
6	T	131	SER
6	T	165	ARG
6	T	181	GLU
6	T	186	ARG
6	T	196	ILE
6	T	201	GLU
6	T	203	ASN
6	T	221	ASN
6	T	243	ILE
7	U	24	LYS
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	120	THR
7	U	166	GLN
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN

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Mol	Chain	Res	Type
8	V	156	SER
8	V	196	ARG
9	W	37	ASN
9	W	52	ILE
9	W	68	TYR
9	W	123	PHE
9	W	166	ILE
9	W	171	LEU
9	W	191	LYS
9	W	202	ARG
10	X	69	ILE
10	X	71	GLU
10	X	92	ILE
10	X	174	MET
10	X	189	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	107	LYS
11	Y	147	ASP
11	Y	211	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	52	MET
12	Z	70	ASN
12	Z	71	SER
12	Z	80	ASN
12	Z	108	HIS
12	Z	109	THR
12	Z	126	ASP
12	Z	132	GLU
12	Z	181	ILE
12	Z	206	ILE
13	a	37	ASN
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	104	ARG
13	a	159	VAL
13	a	161	ARG

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Mol	Chain	Res	Type
13	a	171	GLN
13	a	213	GLN
14	b	6	VAL
14	b	36	ARG
14	b	83	LYS
14	b	88	GLU
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	190	HIS
2	B	20	GLN
2	B	58	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	92	GLN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	233	GLN
3	C	241	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	139	HIS
4	D	146	GLN
4	D	160	ASN

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Mol	Chain	Res	Type
4	D	210	GLN
4	D	217	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	224	HIS
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN
8	H	189	ASN
8	H	219	ASN
9	I	37	ASN
9	I	63	ASN

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Mol	Chain	Res	Type
9	I	71	ASN
9	I	88	GLN
9	I	156	ASN
9	I	203	GLN
10	J	55	GLN
10	J	63	ASN
10	J	65	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
10	J	198	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	208	ASN
11	K	209	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	95	HIS
12	L	108	HIS
12	L	155	ASN
12	L	158	ASN
12	L	159	GLN
12	L	165	ASN
12	L	195	HIS
12	L	197	GLN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	152	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN

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Mol	Chain	Res	Type
14	N	141	ASN
14	N	145	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	93	HIS
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
2	P	232	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	92	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	176	ASN
3	Q	233	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	139	HIS
4	R	146	GLN
4	R	160	ASN
4	R	210	GLN
4	R	217	GLN
4	R	225	ASN
5	S	4	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	GLN

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Mol	Chain	Res	Type
5	S	151	ASN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	83	HIS
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
9	W	71	ASN
9	W	88	GLN
9	W	156	ASN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
10	X	198	GLN

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Mol	Chain	Res	Type
11	Y	9	GLN
11	Y	62	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	95	HIS
12	Z	108	HIS
12	Z	155	ASN
12	Z	158	ASN
12	Z	159	GLN
12	Z	165	ASN
12	Z	195	HIS
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	141	ASN
14	b	145	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LYO	e	3	15	7,9,10	1.10	0	7,10,12	0.98	1 (14%)
15	OW6	d	4	11,15	5,6,7	1.10	0	5,6,8	0.74	0
15	LYO	f	3	15	7,9,10	0.97	0	7,10,12	1.62	1 (14%)
15	OW6	f	4	11,15	5,6,7	1.07	0	5,6,8	0.71	0
15	OW6	c	4	15,8	5,6,7	1.33	1 (20%)	5,6,8	0.70	0
15	OW6	e	4	15,8	5,6,7	1.02	0	5,6,8	0.72	0
15	LYO	c	3	15	7,9,10	1.07	0	7,10,12	0.93	1 (14%)
15	LYO	d	3	15	7,9,10	1.07	0	7,10,12	1.67	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LYO	e	3	15	-	3/8/9/11	-
15	OW6	d	4	11,15	-	1/4/4/5	-
15	LYO	f	3	15	-	3/8/9/11	-
15	OW6	f	4	11,15	-	1/4/4/5	-
15	OW6	c	4	15,8	-	1/4/4/5	-
15	OW6	e	4	15,8	-	1/4/4/5	-
15	LYO	c	3	15	-	3/8/9/11	-
15	LYO	d	3	15	-	3/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	OW6	C17-CA	2.35	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	3	LYO	CB-CA-C	-3.94	104.93	110.99
15	f	3	LYO	CB-CA-C	-3.80	105.14	110.99
15	e	3	LYO	CB-CA-C	-2.34	107.40	110.99
15	c	3	LYO	CB-CA-C	-2.16	107.67	110.99

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	3	LYO	C-CA-CB-CG
15	c	3	LYO	CG-CD-CE-NZ
15	d	3	LYO	C-CA-CB-CG
15	d	3	LYO	CG-CD-CE-NZ
15	e	3	LYO	N-CA-CB-CG
15	e	3	LYO	C-CA-CB-CG
15	e	3	LYO	CG-CD-CE-NZ
15	f	3	LYO	C-CA-CB-CG
15	f	3	LYO	CG-CD-CE-NZ
15	c	4	0W6	CA-C17-C18-C
15	e	4	0W6	CA-C17-C18-C
15	d	4	0W6	CA-C17-C18-C
15	f	4	0W6	CA-C17-C18-C
15	c	3	LYO	N-CA-CB-CG
15	d	3	LYO	N-CA-CB-CG
15	f	3	LYO	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.26	4 (1%) 70 61	44, 65, 95, 118	0
1	O	250/250 (100%)	-0.30	2 (0%) 82 75	43, 66, 96, 118	0
2	B	244/244 (100%)	-0.08	6 (2%) 58 48	45, 67, 107, 132	0
2	P	244/244 (100%)	-0.05	7 (2%) 53 43	46, 68, 107, 133	0
3	C	241/241 (100%)	-0.04	7 (2%) 53 43	48, 71, 119, 140	0
3	Q	241/241 (100%)	0.05	4 (1%) 69 60	49, 74, 120, 140	0
4	D	242/242 (100%)	-0.02	7 (2%) 53 43	50, 72, 105, 139	0
4	R	242/242 (100%)	0.00	5 (2%) 63 54	51, 73, 106, 139	0
5	E	233/233 (100%)	0.09	4 (1%) 69 60	51, 77, 102, 124	0
5	S	233/233 (100%)	0.15	3 (1%) 75 66	50, 77, 103, 124	0
6	F	244/244 (100%)	-0.09	2 (0%) 82 75	47, 67, 103, 117	0
6	T	244/244 (100%)	0.00	2 (0%) 82 75	47, 67, 102, 117	0
7	G	243/243 (100%)	-0.21	2 (0%) 82 75	43, 63, 92, 124	0
7	U	243/243 (100%)	-0.24	2 (0%) 82 75	45, 63, 92, 123	0
8	H	222/222 (100%)	-0.42	0 100 100	41, 57, 79, 118	0
8	V	222/222 (100%)	-0.46	0 100 100	43, 58, 79, 117	0
9	I	204/204 (100%)	-0.52	0 100 100	40, 59, 80, 97	0
9	W	204/204 (100%)	-0.44	0 100 100	40, 59, 81, 97	0
10	J	198/198 (100%)	-0.42	4 (2%) 65 56	41, 57, 77, 137	0
10	X	198/198 (100%)	-0.46	2 (1%) 79 72	42, 58, 78, 137	0
11	K	212/212 (100%)	-0.44	0 100 100	41, 58, 79, 86	0
11	Y	212/212 (100%)	-0.46	0 100 100	40, 58, 80, 87	0
12	L	222/222 (100%)	-0.37	1 (0%) 87 82	41, 60, 84, 108	0
12	Z	222/222 (100%)	-0.34	2 (0%) 81 74	40, 60, 84, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.40	1 (0%) 88 84	39, 59, 76, 83	0
13	a	233/233 (100%)	-0.41	1 (0%) 88 84	39, 58, 76, 82	0
14	N	196/196 (100%)	-0.41	0 100 100	36, 54, 78, 90	0
14	b	196/196 (100%)	-0.45	1 (0%) 87 82	37, 54, 78, 90	0
15	c	1/4 (25%)	0.59	0 100 100	63, 63, 63, 63	0
15	d	1/4 (25%)	0.82	0 100 100	53, 53, 53, 53	0
15	e	1/4 (25%)	1.36	0 100 100	64, 64, 64, 64	0
15	f	1/4 (25%)	-0.68	0 100 100	53, 53, 53, 53	0
All	All	6372/6384 (99%)	-0.24	69 (1%) 78 70	36, 63, 99, 140	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	6.1
7	U	243	ASP	5.4
4	D	119	ALA	5.2
4	D	118	GLY	4.8
4	R	119	ALA	4.4
12	L	174	TYR	4.1
10	X	198	GLN	4.0
13	M	1	THR	4.0
5	S	1	PHE	3.9
2	B	219	ALA	3.9
13	a	1	THR	3.8
10	J	197	ALA	3.6
4	R	124	ARG	3.6
10	J	198	GLN	3.5
2	B	218	GLY	3.5
2	B	244	THR	3.5
4	R	120	SER	3.4
7	G	1	ALA	3.4
3	C	50	LEU	3.3
4	D	120	SER	3.3
3	C	48	SER	3.3
5	E	1	PHE	3.2
3	C	49	THR	3.2
12	Z	174	TYR	3.2
1	A	2	THR	3.2
4	D	124	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
3	Q	52	LEU	3.1
5	E	233	ILE	3.0
2	P	219	ALA	2.9
7	U	1	ALA	2.9
4	R	125	LEU	2.9
4	D	240	ALA	2.8
10	X	1	MET	2.7
6	T	215	CYS	2.7
1	O	2	THR	2.7
6	F	202	ASP	2.7
4	D	121	GLY	2.6
2	P	244	THR	2.6
3	C	53	GLN	2.5
5	E	183	GLY	2.4
1	A	1	MET	2.4
1	O	1	MET	2.4
4	R	118	GLY	2.4
3	Q	231	VAL	2.4
6	F	1	GLY	2.3
3	C	57	ILE	2.3
2	B	1	GLY	2.3
2	B	222	GLY	2.3
1	A	201	GLU	2.3
2	B	220	ASN	2.3
5	E	202	ASP	2.3
2	P	223	GLU	2.2
5	S	2	ARG	2.2
3	C	206	LYS	2.2
12	Z	173	LYS	2.2
2	P	220	ASN	2.1
3	Q	49	THR	2.1
14	b	116	GLY	2.1
10	J	196	GLN	2.1
4	D	125	LEU	2.1
2	P	1	GLY	2.1
3	C	203	THR	2.1
7	G	243	ASP	2.1
5	S	166	GLY	2.0
2	P	60	THR	2.0
6	T	178	HIS	2.0
1	A	249	ALA	2.0
2	P	59	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
10	J	11	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	LYO	e	3	10/11	0.87	0.13	60,61,62,63	0
15	OW6	c	4	7/8	0.90	0.12	57,58,61,63	0
15	OW6	e	4	7/8	0.90	0.13	57,59,61,62	0
15	LYO	d	3	10/11	0.92	0.10	48,51,53,54	0
15	LYO	c	3	10/11	0.92	0.11	59,60,63,63	0
15	LYO	f	3	10/11	0.93	0.09	48,51,53,54	0
15	OW6	f	4	7/8	0.93	0.10	49,50,56,56	0
15	OW6	d	4	7/8	0.96	0.09	49,50,56,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.